201-12930

skrixer@chemintox.com on 01/26/2001 08:12:08 PM

To: NCIC OPPT/DC/USEPA/US@EPA, hpv.crtk@epamail.epa.gov, Rtk Chem/DC/USEPA/US@EPA
cc: tadams@chemintox.com

Subject: Submission of Test Plan and Robust Summaries from FFHPVC

ORIGINAL

Dear Ms. Browner:

On behalf or the member companies of the Terpene Consortium, the Flavor and Fragrance High Production Volume Consortia is pleased to submit the Test Plan and Robust Summaries for the chemical category designated the "Tertiary Terpenoid Alcohols and Related Esters" to the HPV Challenge Program, AR-201. The Terpene Consortium has chosen not to belong to the HPV Tracker System for submission of test plans and robust summaries. We are therefore submitting the test plan and accompanying robust summaries directly to EPA to make available to the public.

This submission includes one electronic copy in pdf. format and one hard copy. The EPA registration number for the Terpene Consortium is 1101125.

Please feel free to contact me with any questions or comments you might have concerning the submission at tadams@therobertsgroup.net, tadams@chemintox.com or 202-331-2325.

Respectfully,
Timothy B. Adams, Ph. D.
Technical Contact Person FFHPVC

Thanks,

Sue

- Submission Letter for Tertiary Alcohol Category.pdf
- Test Plan Terp Tert Alc Est.pdf
- Robust Summaries Terp Tert Alc Est.pdf

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The Flavor and Fragrance High Production Volume Consortia (FFHPVC)

1620 I Street, N.W.
Suite 925
Washington D.C. 20006
Tel. (202)-293-5800 Fax (202)-463-8998

January 26, 2001

Carol Browner, Administrator
US EPA
P.O. Box 1473
Merrifield, VA 22116
Attn: Chemical Right-to-Know Program

Dear Ms. Browner:

On behalf or the member companies of the Terpene Consortium, the Flavor and Fragrance High Production Volume Consortia is pleased to submit the Test Plan and Robust Summaries for the chemical category designated the "Tertiary Terpenoid Alcohols and Related Esters" to the HPV Challenge Program, AR-201. The Terpene Consortium has chosen not to belong to the HPV Tracker System for submission of test plans and robust summaries. We are therefore submitting the test plan and accompanying robust summaries directly to EPA to make available to the public.

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Please feel free to contact me with any questions or comments you might have concerning the submission at tadams@therobertsgroup.net, tadams@chemintox.com or 202-331-2325.

Sincerely,

Timothy Adams, Ph.D.
Technical Contact Person for FFHPVC

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AR 201-12930A

The Flavor and Fragrance High Production Volume Consortia

The Terpene Consortium

Test Plan for Terpenoid Tertiary Alcohols and Related Esters

Linalool (3,7-dimethyl-1,6-octadien-3-ol)	CAS No. 78-70-6
Tetrahydrolinalool (3,7-dimethyl-3-octanol)	CAS No. 78-69-3
Myrcenol (2-methyl-6-methylene-7-octen-2-ol)	CAS No. 543-39-5
Dihydromyrcenol (3,7-dimethyl-7-octen-2-ol)	CAS No. 18497-58-8
Linalyl acetate (3,7-dimethyl-1,6-octadien-3-yl acetate	CAS No. 115-95-7
alpha-Terpineol (*p*-menth-1-en-8-ol)	CAS No. 98-55-5
alpha-Terpinyl acetate (*p*-menth-1-en-8-yl acetate)	CAS No. 80-26-2
2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products, linalool fractions, acid-isomerized, distn. residues, acid-isomerized, distn. lights, terpenoids	CAS No. 125252-49-5
cis-2-Pinanol	CAS No. 4948-28-1
2-Pinanol	CAS No. 473-54-l
trans-2-Pinanol	CAS No. 4948-29-2
2-Pinanol hydroperoxide	CAS No. 28324-52-9
Pine oil	CAS No. 8002-09-3

FFHPVC Terpene Consortium Registration Number

Submitted to the EPA under the HPV Challenge Program by:

The Flavor and Fragrance High Production Volume Chemical Consortia

1620 I Street, NW, Suite 925

Washington, DC 20006

Phone: 202-331-2325

Fax: 202-463-8998

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List of Member Companies

Sponsoring Substances in Tertiary Terpenoid Alcohols and Related Ester Derivatives

Arizona Chemical

BASF

Bush Boake Allen, Inc.

Citrus and Allies Essences, LTD

Givaudan Roure

ICI Americas

International Flavors and Fragrances Inc.

J. Manheimer Incorporated

Hercules Chemical

Millennium Chemicals, Inc.

TECNAL Corporation

Universal Flavor Corporation

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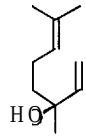
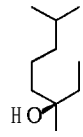
The HPV Challenge Test Plan for Tertiary Terpenoid Alcohols and Related Esters

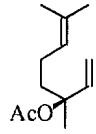
1 Identity of Substances



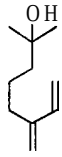
3,7-Dimethyl-1,6-octadien-3-ol
Linalool
$C_{10}H_{18}O$
CAS No. 78-70-6



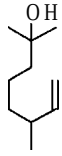
3,7-Dimethyloctan-3-ol
Tetrahydrolinalool
$C_{10}H_{22}O$
CAS No. 78-69-3



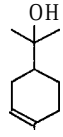
3,7-Dimethyl-1 ,6-octadien-3-yl acetate
Linalyl acetate
$C_{12}H_{20}O_2$
CAS No. 115-95-7



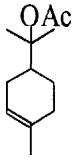
2-Methyl-6-methylene-7-octen-2-ol
Myrcenol
$C_{10}H_{18}O$
CAS No. 543-39-5



2,6-Dimethyl-7-octen-2-ol
Di hydromyrce nol
$C_{10}H_{20}O$
CAS No. 18479-58-8

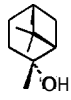


p-Menth-1-en-8-ol
alpha-Terpineol
$C_{10}H_{18}O$
CAS No. 98-55-5



p-Menth-1-en-8-yl acetate
alpha-Terpineol acetate
$C_{10}H_{20}O_2$
CAS No. 80-26-2

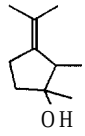
cis-2-Pinanol
$C_{10}H_{18}O$
CAS No. 4948-28-1



trans-2-Pinanol
$C_{10}H_{18}O$
CAS No. 4948-29-2

2-Pinanol
$C_{10}H_{18}O$
CAS No. 473-54-l

2-Pinanol hydroperoxide
Pinane hydroperoxide
$C_{10}H_{18}O_2$
CAS No. 28324-52-9



2,6,6-Trimethylbicyclo
[3. 1.1]heptan-2-ol thermal rearrangement products
CAS No. 125252-49-5
Major isomer: plinol
$C_{10}H_{18}O$
CAS No. 72402-00-7

2 Category Analysis

2.1 Introduction

In October of 1999, members of the U.S. flavor and fragrance industries as well as other manufacturers that produce source materials used in flavors and fragrances formed consortia of companies in order to participate in the Chemical Right-to-Know Program. Members of these consortia are committed to assuring the human and environmental safety of substances used in flavor and fragrance products. The consortia are organized as the Flavor and Fragrance High Production Volume Consortia (FFHPVC). The Terpene Consortium, as a member of FFHPVC serves as an industry consortium to coordinate testing activities for terpenoid substances under the Chemical Right-to-Know Program. Seventeen (17) companies are current members of The Terpene Consortium, twelve (12) of which are sponsoring substances in this chemical category. The Terpene Consortium and its member companies are committed to assembling and reviewing available test data, developing and providing test plans for each of the sponsored chemicals, and, where needed, conducting additional testing. The category analysis, test plan, and robust summaries presented represent the first phase of the Consortium's commitment to the Chemical Right-to-Know Program.

2.2 Background Information

In nature terpenes are produced by the isoprene pathway, which is an integral part of normal plant and animal biosynthesis. They are ubiquitous in the environment and in food consumed by humans and other animals. Linalool and alpha-terpineol are two of the most common terpenoid alcohols, occurring to varying degrees in essentially all plants [Lawrence, 1985]. Linalool accounts for more *than 70%* of *the* spice essential oil, coriander oil. A mixture of *alpha*-terpineol and its acetate ester, linalool and its acetate ester, and other tertiary terpenoid alcohols account for more than 70% of cardamom oil [Gopalaluishnan and Narayan, 1991]. Linalool and *alpha-terpineol, the* two parent alcohols in this category, are widely dispersed in fruits and vegetables as well as the fermented products prepared from these foods. Principal exposure to

these two terpenes arises via the consumption of spices, carrots, orange juice, nutmeg, beer, wine, and tea [Stofberg and Grundschober, 1987]. Ten (10) of the 13 substances in this chemical category are currently recognized by the US. Food and Drug Administration (FDA) as GRAS ("generally regarded as safe") for their intended use as flavoring substances [Hall and Oser, 1965]. However, quantitative data on natural occurrence indicate that oral intake of these substances occurs predominantly from consumption of food in which they occur naturally [Stofberg and Grundschober, 1987; Stofberg and Kirschrnan, 1985]. For example, greater than 200,000 pounds (lbs) of linalool and alpha- terpineol, and their corresponding acetate esters are consumed annually as natural components of traditional foods not including spices [Stofberg and Grundschober, 1987]. Including the consumption of spice and spice oils, intake of these alcohols exceeds 1,000,000 lbs annually [Lawrence, 1985]. On the other hand, the intentional use of these materials in flavors results in the annual consumption of less than 50,000 lbs [Lucas ***et al.,*** 1999].

2.3 Structural Classification

The chemical category designated "Tertiary Terpenoid Alcohols and Related Esters" includes eight terpenoid aliphatic tertiary alcohols and two related acetate esters. The group of alcohols consist of linalool (3,7-dimethyl- 1,6-octadien-3-ol), tetrahydrolinalool (3,7-dimethyl-3-octanol), a tertiary alcohol isomer of linalool, myrcenol (2-methyl-6-methylene-7-octen-2-ol), dihydromyrcenol (3,7-dimethyl-7-octen-2-ol); ***an*** isomeric alicyclic tertiary alcohol *alpha*-terpineol (*p*-menth- 1 -en-8-ol), 2-pinanol, and ***cis***- and *trans*-2-pinanol. The two esters include the acetate ester of linalool (3,7-dimethyl- 1,6-octadien-3-yl acetate) and acetate ester of ***alpha-terpineol*** (*p*-menth- 1-en-8-yl acetate).

This chemical category also includes a site-restricted peroxide of a terpene tertiary alcohol (pinane hydroperoxide) that is efficiently reduced to the corresponding alcohol (2-pinanol). It also includes two mixtures consisting predominantly of tertiary terpenoid alcohols. These two mixtures are pine oil and "2,6,6-trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement

products, linalool h-actions, acid-isomerized distillation residues, acid-isomer&d distillation lights, terpenoids". The composition of these mixtures is discussed below.

Seven of the ternary alcohols are isomers of the formula $C_{10}H_{18}O$, one is a dihydro homologue ($C_{10}H_{20}O$), and one is a tetrahydro homologue ($C_{10}H_{22}O$). The two acetate esters have the formula $C_{12}H_{20}O_2$. The pinane hydroperoxide has the formula $C_{10}H_{18}O_2$. The two mixtures are composed principally of terpenoid tertiary alcohols of the formula $C_{10}H_{18}O$.

2.3.1 Pinane hydroperoxide

Pinane hydroperoxide is a mixture of approximately 75% *cis*- and 25% *trans*-isomers [Canova, 1977]. Commercially it is a site-restricted chemical intermediate, which is formed by the oxidation of ***alpha-pinene*** with molecular oxygen. The vast majority of industrial pinane hydroperoxide is reduced with sodium bisulfite or other reducing agents to yield mixtures of the commercially important alcohols, *cis*-2-pinanol (55-56%) and *trans*-2-pinanol (25-27%). Small amounts of terpene hydrocarbons (limonene, ***alpha-*** and beta-pinene, menthene) and other terpenoid alcohols ***(alpha-terpineol,*** isopinocampheol, isoverbanol, bomeol) are also formed [Gorman, 1976; Brose et ***al.,*** 1992]. ***Cis-*** and *trans*-2-pinanol are then separated and thermally converted to (+)-linalool and (-)-linalool, respectively.

Pinane hydroperoxide is a relatively stable peroxide with a shelf half-life greater than 100 hours at 120°C. During transportation it is recommended that the peroxide be stored in tightly closed containers at temperatures less than 35°C [Millennium Specialty Chemicals, 1999]. In addition to being a source of *cis*-2-pinanol and *trans*-2-pinanol, pinane hydroperoxide acts as a polymerization initiator in the production of vinyl, nitrile, styrene-butadiene, and polyester resins [Millennium Specialty Chemicals, 1999]. Similar to other tertiary aliphatic peroxides, pinane hydroperoxide [Milas and Surgenor, 1946] undergoes decomposition to yield 2-pinanol and other terpenoid alcohols. To a minor extent, it rearranges via alpha-cleavage to form ketones [Schmidt and Fisher, 1959].

2.3.2 Pine oil

Although a minor amount of commercial pine oil is still derived from natural sources (i.e., pine trees), the vast majority of pine oil in use today is synthetic in nature. Originally, pine oil was obtained by the steam distillation of crude turpentine from pine trees, mainly stumps rich in terpene oils. Today, it is produced predominantly by acid-catalyzed hydration of pinene. The definition of pine oil reflects its isolation from natural sources. According to the Toxic Substances Control Act [TSCA-PL 94-469, Addendum III, Chemical Substances of Unknown or Variable Composition, 1978] pine oil is defined as "a complex combination of terpenes produced by high temperature distillation of oil of turpentine residues or by catalytic hydration of pinene. It is composed primarily of tertiary and secondary terpene alcohols."

The composition of pine oil obtained by steam distillation varies depending on pine tree feed stocks and processing. The major constituent, alpha-terpineol (8-terpineol) accounts for 50-60% of the oil by weight. Other tertiary terpenoid alcohols, such as 1- and 4-terpineol, account for 15-25% of the oil with the remainder being composed of terpene hydrocarbons (5- 10%), secondary terpenoid alcohols, mainly fenchol and bomeol (5-10% each), terpene ethers (5-10%), ketones, and phenols (1-2%). High-grade natural pine oil may contain as much as 70% alpha-terpineol [Guenther, 1952].

The composition of synthetic pine oil derived from hydration of pinene is also predominantly composed of tertiary terpenoid alcohols. Specifically, the composition of pine oil used in toxicologic studies performed from 1990- 1991 was a blend of commercial oils from six major pine oil producers [Davis, 2000]. Multiple batch independent analysis [Toxikon, Inc., 1990] of this blend was found to contain 56.2% alpha-terpineol, 9.2% gamma-terpineol, 4.3% other terpineols (beta-terpineol, 4-terpineol), 6.5% secondary terpenoid alcohols (fenchol and bomeol), 20.4% terpene hydrocarbons (mainly limonene, p-menthadiene, and terpinolene), and <4% of aromatic and alicyclic terpene hydrocarbons and ethers. In addition to alpha-terpineol, some grades of commercial pine oil may also contain minor amount of *cis* and *trans*-2-pinanol, alpha-terpineol acetate, and linalool [Millennium Specialty Chemicals, 2000]. The pine oil blend

used in toxicity studies performed in 1994 consisted of 62.7% alpha-terpineol and 83.4% total terpene alcohols [Villa, 1994]. Pine oil was blended from five commercially available lots of pine oil and subjected to toxicity studies from 1985-1987. The range of concentrations of terpene constituents in the five lots contained 35- 76.7% ***alpha-*** and gamma-terpineol, 1- 13.1% other terpineol isomers, 0- 14.6% secondary terpene alcohols, 0. 1- 10% terpene hydrocarbons [Hercules, 200 1].

Prior to 1970, toxicology studies were performed on commercial grades of pine oil commonly recognized as Yarmor. Similar to commercial grades of pine oil available today, Yarmor contains 50-60% alpha-terpineol in combination with other terpineols (10- 15%), linalool (1%), secondary terpenoid alcohols (7-15%), and terpene hydrocarbons (10-20%) [CSMA, 2000]. Based on these data, it can be concluded that commercial pine oil and pine oil subjected to toxicity studies is composed of 60-80% terpineol isomers, ***mainly the alpha*** isomer. The remaining constituents are primarily secondary terpenoid alcohols and terpene hydrocarbons.

2.3.3 2,6,6-Trimethylbicyclo[3.1 .1]heptan-2-ol - thermal rearrangement products

The rearrangement products from thermolysis of pinanol (2,6,6-trimethylbicyclo [3.1. 1]heptan-2-ol) include plinol (1,2-dimethyl-3-isopropenylcyclopentanol, 47-50%), *trans*-2-pinanol (2 1-24%), linalool (7-9%), *cis-beta*-terpineol (1-2%), *p*-menthan- 1-ol (1-2%) and the secondary bicyclic alcohol alpha-fenchol (<4%). The remaining components each of which accounts for less than 1% of the mixture are simple aliphatic alcohols and terpenoid hydrocarbons (geraniol, myrcene, limonene, and alpha-pinene) [Millennium Specialty Chemicals, 2000]. The major isomer plinol (CAS No. 72402-00-7) is a tertiary alcohol and is structurally related to *alpha*-terpineol. Because of its ready hydrolysis to plinol, plinyl acetate (1,2-dimethyl-3-isopropenylcyclopentanyl acetate) is considered a good closely related structural model for this product.

The thirteen substances are assigned to the same chemical category because of their close structural relationships, their similar physio-chemical properties, including the ready conversion of linalool to alpha-terpineol. They are also considered together by virtue of the fact that they

participate in the same pathways of metabolic detoxication and have similar toxicologic potential.

2.4 Industrial and Biogenic Production

2.4.1 Industrial Production

(+/-)-Linalool and its esters are the most frequently used in fragranced products. However, most of the manufactured linalool is used in the preparation of Vitamin E. Like its enantiomers, the racemic form (+/-)-linalool provides a flowery-fresh fragrance, reminiscent of lily of the valley. Although it can be isolated from essential oils such as Brazilian rosewood oil, most linalool used in fragrances and flavors is produced synthetically. Preparation from alpha-pinene via pinane hydroperoxide selectively yields the optically active (+) and (-) forms of linalool [Canova, 1977]. An alternate synthesis involves sequential conversion of beta-pinene to myrcene, which in turn, is converted to linalyl chloride in the presence of HCl and copper (I) catalysts. The chloride is then converted to linalyl acetate, which may be used as is or saponified to linalool [Webb, 1964].

Myrcenol is prepared from myrcene by addition of HCl, followed by hydrolysis [Blumenthal, 1966]. Likewise, dihydromyrcenol is formed from hydrohalogenation and hydrolysis of 2,6-dimethyl-2,7-octadiene, a thermal degradation product of *cis*-pinane [Webb, 1960]. Tetrahydrolinalool is prepared by the catalytic hydrogenation of linalool.

alpha-Terpineol is a highly important commercial product. Only small quantities are isolated from essential oils. An efficient synthesis involves the simple hydration of pinene from turpentine to yield *cis*-terpin hydrate followed by dehydration to yield alpha-terpineol [Hoyer et *al.*, 1959]. Selective hydration of pinene, delta-3-carene, and limonene or diterpene is also used to generate alpha-terpineol. The tertiary terpenoid alcohols *cis*- and *trans*-2-pinanol are synthesized from pinane via the hydroperoxide.

Commercially, the use of pine oil exceeds the annual use of all other members of this chemical category. Annual industrial production of pine oil is approximately 30,000,000-35,000,000 lbs of which only 4,000,000 to 5,000,000 lbs is derived from distillation of naturally occurring sources, mainly crude sulfate turpentine. The remainder is a synthesized product using pinene as a source material [PSMA, 2000]. Production of pine oil has changed significantly during the last half decade. Whereas synthetic pine predominates in the current marketplace, essentially all of the roughly 8,000,000 lbs of pine oil produced in 1950- 195 1 came from the distillation of crude turpentine [Goldblatt, 195 1].

2.4.2 Biogenic Production

Linalool, myrcenol, alpha-terpineol, and their related esters, homologues, and mixtures are common plant monoterpenoids that are ubiquitous in the environment. Most if not all vegetation produces these alcohols and esters. Environmental monitoring has detected ambient atmospheric [Larsen *et al.*, 1997] and aquatic [Heil and Lindsay, 1990] levels of tertiary terpenoid alcohols, The environmental impact of these substances must consider not only industrial sources and emissions, but also biogenic sources and emissions. Arguably, if background biogenic production and subsequent emission of terpenoid alcohols exceeds industrial (anthropogenic) production and emission by orders of magnitude, no significant environmental impact from industrial use and production can be expected.

Linalool, alpha-terpineol, myrcenol, and their corresponding acetate esters are present in almost every conceivable plant. Therefore, daily consumption of fresh fruit and vegetables and processed foods and drinks derived from these food groups provides exposure to these substances. Estimates of consumption of these substances as the result of food consumption exceeds 200,000 lbs annually [Stofberg and Grundschober, 1987]. This value represents a minute fraction of the biogenic production of these substances in the environment. For instance, consider the biogenic stores and biogenic production of tertiary terpenoid alcohols from pine trees, Based on the known relative amount of pine oil (tertiary terpenoid alcohols, mainly *alpha*-terpineol) in steam distilled wood turpentine obtained from longleaf and slash pine in the Eastern

U.S.A, it is possible to estimate the amount of these tertiary alcohols released from pine sources. One ton of air seasoned dry "fat" wood yields approximately 4 gallons or 14 lbs of pine oil, which is made up of approximately 10 lbs of tertiary terpenoid alcohols [Guenther, 1952]. One acre produces approximately 5 tons of viable pine stumps, the part of the tree richest in sources of turpentine and pine oil. Therefore approximately 50 lbs of tertiary alcohols are available per acre or 1,000,000,000 lbs for 20,000,000 acres of pine-forested land in the U.S.A. Although this simplified estimate is both crude and limited, it provides a perspective on the potential sources of tertiary terpenoid alcohols available from the environment.

2.5 Hydrolysis in Aqueous Media

The two terpenoid esters in this chemical category can be hydrolyzed to their corresponding terpenoid alcohol and acetic acid. Hydrolysis can be catalyzed by classes of enzymes recognized as carboxylesterases or Btype esterases [Heymann, 1980] that predominate in hepatocytes [Heymann, 1980]. Terpenoid alcohols formed in the gastrointestinal tract are rapidly absorbed [Phillips et *al.*, 1976; Diliberto *et al.*, 1988]. During hydrolysis under acidic conditions linalool may cyclize to form *alpha-terpineol* [Buck and Renwick, 1998; Buck and Renwick, 1999].

The esters of linalyl acetate and alpha-terpineol acetate are hydrolyzed under various *in vitro* and *in vivo* conditions *to* yield linalool or *alpha-terpineol*, respectively, and acetic acid. In an *in vitro* hydrolysis study, linalyl acetate was easily hydrolyzed in water, simulated gastric juice (pH 1.8), and pancreatic fluids (pH 7.5) [Buck and Renwick, 1999]. The mean half-lives for linalyl acetate hydrolysis in gastric juice with and without added hydrolytic enzymes was less than 2.5 minutes, respectively. Mean half-lives were less than 100 minutes in intestinal fluids in the absence or presence of pancreatin [Buck and Renwick, 1999]. Linalyl acetate also hydrolyzed in homogenates of rat intestinal mucosa, blood, and liver, but at rates much slower than in acidic gastric juice (rate constant for hydrolysis $k=0.01$ to 0.0055 min^{-1} versus greater than 5 min^{-1} in gastric juice). alpha-Terpineol acetate is also rapidly hydrolyzed in simulated gastric juice. The mean half-life in gastric juice is reported to be 16.4 minutes. In intestinal fluid (pH 7.5)

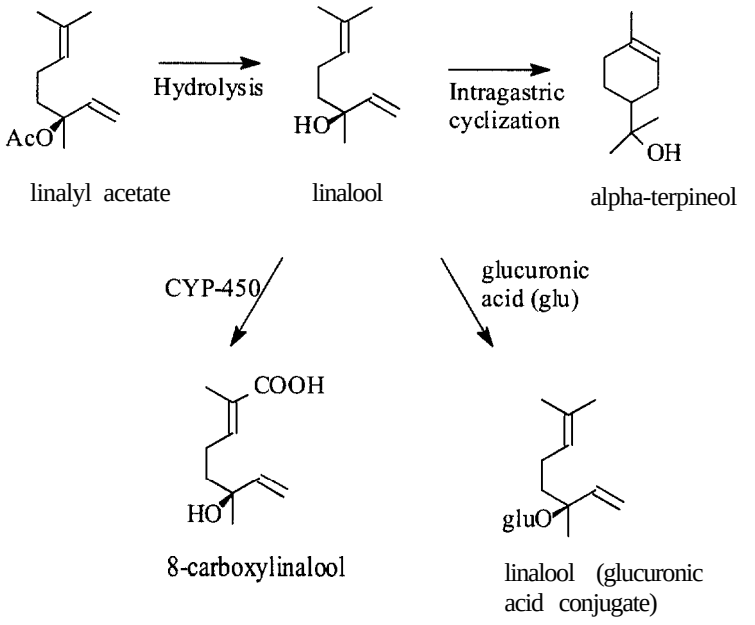
hydrolysis is somewhat slower (mean half-live, less than 400 minutes) [Buck and Renwick, 1999].

Carboxylesterase (Type B) activity also has been reported in a variety of fish species at different life stages [Leinweber, 1987; Boone et al., 1996; Abas and Hayton, 1997; Barr-on et ***al.,*** 1999]. Enzyme activity of rainbow trout sera, liver and whole body homogenates were similar to those of rat liver homogenate. A significant increase (300%) in activity occurred between yolk-sac and juvenile stage of rainbow trout development. Carboxylesterase activity was not significantly different for whole body homogenates of the rainbow trout, channel catfish, fathead minnows, and bluegill [Barron et ***al.,*** 1999]. These data support the conclusion that simple terpenoid esters, including linalyl acetate and alpha-terpineol acetate, are readily hydrolyzed in fish.

2.6 Reactivity in Aqueous Media

Following hydrolysis of linalyl acetate, resulting linalool partially undergoes ring closure to yield mainly alpha-terpineol and minor amounts of the terpenoid primary alcohols, geraniol and nerol (see Figure 1). In acidic (pH 1.8) artificial gastric juice, linalyl acetate is rapidly hydrolyzed ($t_{1/2}$<2.5 min.) to yield linalool. In neutral media (pH 7.5), hydrolysis is slower ($t_{1/2}$= <100 min.). Under both conditions of pH, approximately one-third of the resulting linalool is then rapidly rearranged to yield alpha-terpineol and small amounts of geraniol and nerol [Buck and Renwick, 1998; Buck and Renwick, 1999]. Based on these observations it can be concluded that linalyl acetate hydrolyzes under acidic conditions (i.e., gastric juice) to yield linalool which, to some extent, undergoes cyclization to yield ***alpha-terpineol.*** Both linalool and *alpha*-terpineol may then be either conjugated and excreted or oxidized to more polar excretable metabolites (see discussion below).

Figure 1. Metabolism of Linalool in Mammals



2.7 Metabolism of Tertiary Terpenoid Alcohols

In humans and animals, terpenoid tertiary alcohols primarily conjugate with glucuronic acid and are excreted in the urine and feces [Homing *et* al., 1976; Ventura *et* al., 1985; Parke *et* al., 1974a, 1974b; Williams, 1959]. Terpenoid alcohols with unsaturation may also undergo allylic oxidation to form polar diol metabolites that may be excreted either free or conjugated. If the diol contains a primary alcohol function, it may undergo further oxidation to the corresponding carboxylic acid [Madyastha and Srivatsan, 1988; Homing *et al.,* 1976; Ventura *et al.*, 1985].

The metabolic fate of the aliphatic tertiary alcohol linalool has been studied in mammals (see Figure 1). In rat liver homogenate, linalool or its CYP-450 oxidized metabolite is rapidly conjugated with glucuronic acid (t½ for linalool=23 min.). Linalool undergoes rapid oxidation (t½ for linalool=ll min.) in activated CYP-450 rat liver homogenate [Buck and Renwick,

1998]. Linalool, labeled with ^{14}C in positions 1 and 2, was orally administered to rats at a single dose of 500 mg/kg bw. The majority (55%) of the radioactivity was excreted in the urine as the glucuronic acid conjugate of linalool, while 23% was excreted as CO_2 in expired air, and 15% was excreted in the feces within 72 hours of dose administration. Only 3% of the radioactivity was detected in tissues after 72 hours, with 0.5% in the liver, 0.6% in the gut, 0.8% in the skin and 1.2% in the skeletal muscle [Parke et ***al.,*** 1974a] (see Figure 1). Reduction metabolites such as dihydro- and tetrahydrolinalool have been identified in the urine after administration of a single dose of linalool to rats [Rahman, 1974].

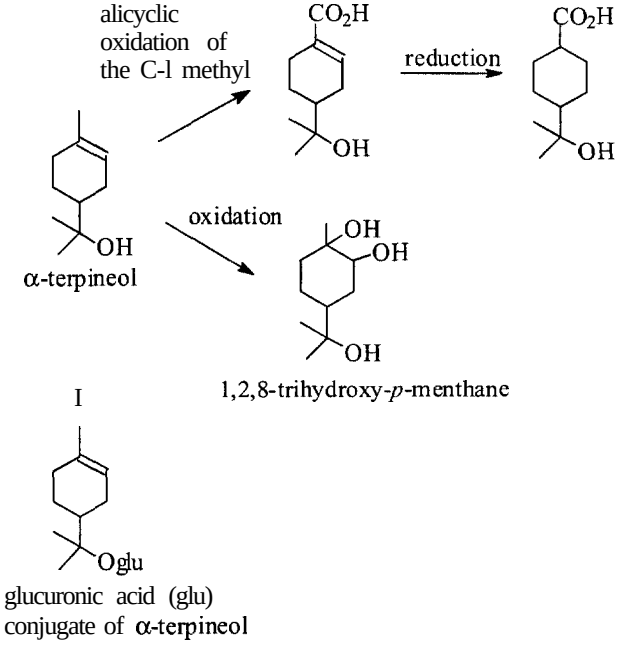
In a separate study, male rats (IISc strain) were given a daily 800 mg/kg bw oral dose of linalool for 20 days. Urinary metabolites formed by cytochrome P-450 (CYP450)-induced allylic oxidation of linalool included 8-hydroxylinalool and 8-carboxylinalool. CYP450 activity in the liver microsomes was increased approximately 50% after three days, but the activity decreased to control values after six days [Chadha and Madyastha, 1984]. Linalool administered daily to 4-week-old male Wistar rats by gavage at a dose of 500 mg/kg bw for 64 days did not induce CYP450 until the 30th day of treatment [Parke et ***al.,*** 1974b].

The data suggest that glucuronic acid conjugation and excretion is the primary route of metabolism of linalool. Allylic oxidation becomes an important pathway only after repeated dosing. It has been suggested that the biotransformation of the diol metabolite of linalool to the corresponding aldehyde via the action of the nicotineamide adenine dinucleotide (NAD+) dependent enzyme alcohol dehydrogenase (ADH) is inhibited due to the bulky nature of the neighboring alkyl substituents and the substrate specificity of the enzyme [Eder et ***al.,*** 1982].

In a repeated dose study, male albino rats (IISc strain) were orally administered the alicyclic tertiary alcohol alpha-terpineol at a daily dose of 600 mg/kg bw for 20 days. Oxidation of the allylic methyl group was observed to yield the corresponding carboxylic acid, which to a small extent, was reduced to yield the corresponding saturated carboxylic acid [Madyastha and Srivatsan, 1988] (see Figure 2). alpha-Terpineol orally administered to rats increased the liver

microsomal CYP-450 content and activity of NADPH-cytochrome c reductase [Madyastha and Srivatsan, 1988] suggesting that oxidation is mediated by CYP-450.

Figure 2. Metabolism of alpha-terpineol in rats



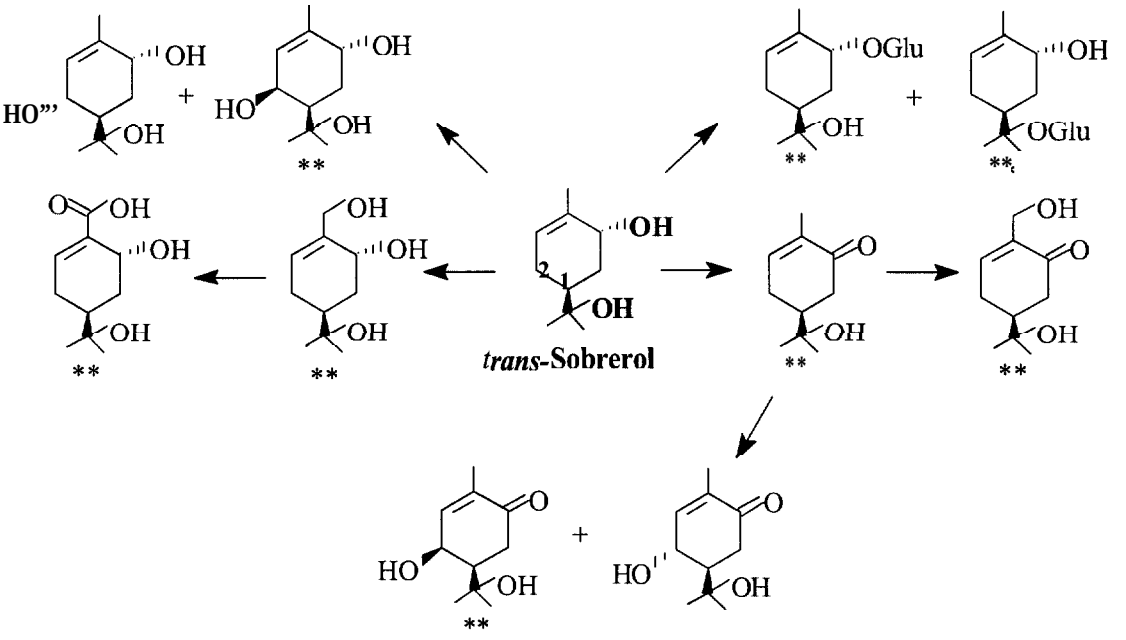
In a minor pathway, the endocyclic alkene of alpha-terpineol is epoxidized and then hydrolyzed to yield a trio1 metabolite 1,2,8-trihydroxy-*p*-menthane which also has been reported in humans following inadvertent oral ingestion of a pine oil disinfectant containing alpha-terpineol [Homing et ***al.***, 1976]. It is expected that after single dose exposures, alpha-terpineol would undergo metabolism like linalool [Chadha and Madyastha, 1984], primarily glucuronic acid conjugation and excretion in the urine.

Bicyclic tertiary alcohols are conjugated with glucuronic acid and excreted primarily in the urine [Williams, 1959]. In rabbits the structurally related bicyclic tertiary alcohols thujyl alcohol (4-

methyl-1-(1-methylethyl)bicyclo[3.1.0]-hexan-3-ol) and beta-santenol (2,3,7-trimethylbicyclo[2.2.1]-heptan-2-ol) are conjugated with glucuronic acid [Williams, 1959].

In a metabolism study using the structurally related terpenoid tertiary alcohol *trans*-sobrerol (see Figure 3), in humans, dogs, and rats, ten metabolites were isolated in urine, eight of which were characterized in humans. Two principle modes of metabolism were observed, allylic oxidation of the ring positions and alkyl substituents, and conjugation of the tertiary alcohol functions with glucuronic acid. These metabolic patterns are common modes of converting tertiary [Ventura *et al.*, 1985] and secondary [Yamaguchi et *al.*, 1994] terpenoid alcohols to polar metabolites, which are easily excreted in the urine and feces (see Figure 3). Menthol forms similar oxidation and conjugation products in rats [Yamaguchi *et al.*, 1994].

Figure 3. Metabolism of *trans*-Sobrerol in Rats, Dogs, and Humans



** Isolated in human urine

In summary, esters of tertiary terpenoid alcohols are readily hydrolyzed in animals, including fish. Once hydrolyzed, the resulting alcohols undergo excretion unchanged or as the glucuronic acid conjugate. To a minor extent, CYP-450 mediated oxidation at the *omega* or *omega*- 1 position yields polar oxidized metabolites capable of excretion primarily in the urine.

2.8 Summary for Category Analysis

Based on the results of hydrolysis, the reactivity of linalool in aqueous media, and data on metabolism it is concluded that members of this chemical category exhibit similar chemical and biochemical fate. The esters are readily hydrolyzed to the corresponding alcohols, linalool and *alpha*-terpineol. Linalool is then partial converted to alpha-terpineol mainly under acidic conditions. Alicyclic and aliphatic tertiary alcohols are efficiently detoxicated by two principal pathways: conjugation primarily with glucuronic acid and excretion primarily in urine, and omega-oxidation to eventually yield diacids and their reduced or hydrated analogs. These polar metabolites will be efficiently excreted primarily in the urine either unchanged or as the glucuronic acid conjugates. The physiochemical and toxicological properties of these substances are consistent with their known reactivity and common metabolic fate.

3 Test Plan

3.1 Chemical and Physical Properties

3.1 .1 Melting Point

All the substances in this chemical category are liquids at ambient temperature. Calculated melting points indicate that alcohols and esters in this category would solidify below 23 °C [SRC]. The melting point of linalool is reported to be less than 20 °C [Givaudan Roure, 1991a] and the solidification temperature of the *d* and *l* forms of alpha-terpineol are reported to be 3 1 and 34.4 °C, respectively [SRC; Merck Index, 1997].

3.1.2 Boiling Point

Members of this chemical category are branched-chain acyclic or alicyclic tertiary alcohols and related esters. The molecular weights of the alcohols are within a narrow range (154 to 158 daltons). Therefore, it is not unexpected that their experimentally determined boiling points are also within a narrow range (196-230 "C). The alicyclic alcohols (e.g., alpha-terpineol) show slightly higher boiling points than their acyclic counterparts (e.g., myrcenol and linalool).

While only one of the reported boiling points was obtained according to a recent ASTM guideline, the consistency of the values reported by the Fragrance Materials Association (FMA) and standard reference sources (Merck Index, 1997) confirms their reliability. Linalool and plinol acetate (the corresponding ester of the major component of pinanol thermal rearrangement products) show relatively low boiling points of 198 [FMA] and 196 °C [Lurnsden, 1998], respectively, while alpha-terpineol exhibits a boiling point of 217-2 18 °C [FMA, FOA]. *cis*- and *trans*-Pinanol exhibit nearly identical boiling points (205-206 °C at 1 atmosphere pressure) [FMA]. The boiling point of pine oil, which is a mixture of mainly tertiary terpenoid alcohols, is in the range of 200-220 °C [FMA]. No boiling point is reported for the site-restricted peroxide pinane hydroperoxide. As a chemical intermediate, this thermally unstable substance is maintained at temperatures below 35 "C.

3.1.3 Vapor Pressure

The reported vapor pressures for linalool (0.05 mm Hg, 20 °C [Vuilleumeir et al., 1995] and 0.16 mm Hg (22-25 °C [Misra *et al.*, 1995]), alpha-terpineol (0.04 mm Hg, 22-25 °C [Misra *et al.*, 1995], and plinol 0.02 mm Hg, 22-25 °C [Misra *et al.*, 1995]) correlate well with calculated vapor pressures [FMA; SRC]. The calculated vapor pressure for all alcohols and esters in this group at 20 °C are in the range from 0.02 to 0.12 mm Hg [FMA]. No vapor pressure is reported for the site-restricted peroxide pinane hydroperoxide that is maintained in sealed containers at temperatures below 35 °C.

3.1.4 Octanol/Water Partition Coefficients

Measured log Kow values are available for four substances in this chemical category. Three alcohols, linalool, alpha-terpineol, and plinol exhibit log Kow values of 2.9 [Givaudan Roure, 1991b], 2.98 [Misra *et al.*, 1995], and 2.87 [Misra *et al.*, 1995], respectively. Higher log Kow values of 4.3 [Givaudan Roure, 1996a] and 4.09 [Lumsden, 1998] were reported for the more non-polar acetate esters, alpha-terpineol acetate and the related plinyl acetate, respectively.

The calculated log Kow values as reported by Syracuse Research Corporation (SRC), for eight tertiary terpenoid alcohols in this category are in the range from 2.87 to 3.47, are consistent with experimentally measured values (2.9 and 2.98). Likewise, calculated Kow values of 3.46 and 4.34 for linalyl acetate and *alpha-terpineol* acetate, respectively, agree with measured data for linalyl acetate (log Kow 2.9 [Proctor & Gamble, 1996]), alpha-terpineol acetate (log Kow=4.3 [Givaudan Roure, 1996a]) and for the structurally related ester, plinyl acetate (log Kow=4.09 [Lumsden, 19981).

3.1.5 Water Solubility

While the reported water solubilities were not obtained according to OECD guidelines, the solubility values increase with increased temperature and follow the same trend as measured partition coefficients. The values reported for linalool and alpha-terpineol at 4-8 °C (560 and

341 mg/L, respectively) and at 22-25 °C (867 and 716 mg/L, respectively) [Misra et al., 1995] show an expected increase in solubility. The value for linalool at 22-25 °C is consistent with the value reported for linalool at 20 °C (1450 mg/L) [Givaudan Roure, 1991a] and tetrahydrolinalool (700 mg/L, temperature not specified) [BBA, 1990]. The decreased solubility expected for esters in this category is realized with a solubility of 60.5 mg/L for plinyl acetate obtained from a recent GLP study [Lumsden, 1998] and 140 mg/L at 20 °C for linalyl acetate [Givaudan Roure, 1991 c]. Calculated values (ESPKOW) for the alcohols and esters in this category are in the range from 160 to 863 mg/L and less than 10 mg/L, respectively. The solubility of *cis*-, *tram*-, and unspecified 2-pinanol should exhibit essentially identical water solubilities (see robust summary for *cis*-2-pinanol).

3.1.6 New testing required

None

3.2 Environmental Fate and Pathways

3.2.1 Photodegradation

The calculated photodegradation half-lives for the ternary terpenoid alcohols and esters in this chemical category, are in the range fi-om 1.07 to 9.08 hours [AOPWIN]. Half-lives for alcohols (i.e., linalool and myrcenol) that contain a more reactive allyl alcohol moiety group are shorter than their saturated counterparts (*i.e.*, tetrahydrolinalool and dimyrcenol). Generally, more stable ternary alcohols in this category have longer half-lives than those for more reactive primary terpenoid alcohols (*i.e.*, citronellol, geraniol and nerol half-lives, 19 minutes to 1.3 hours). Calculated half-lives for linalool and alpha-terpineol(l.07 and 1.24 hours, respectively) are in the same range as their corresponding esters (1.10 and 1.35 hours, respectively). The decreased chemical reactivity of these tertiary alcohols, as compared to that of primary terpenoid alcohols, supports slightly longer photodegradation half-lives as predicted by the model.

The photodegradation model was not applied to the two mixtures in this chemical category. These mixtures are composed of tertiary alcohols and esters in this chemical category. As such, the photodegradation of the mixture is represented by the calculated photodegradation rates of its component alcohols and esters. Likewise, *cis*-, *trans*-, and unspecified 2-pinanol should exhibit nearly identical rates of photodegradation (see photodegradation robust summary for *cis*-2-pinanol).

3.2.2 Stability in Water

Hydrolysis data is available for the two acetate esters in this chemical category. Although hydrolysis is not possible for the tertiary alcohols in this category, it is possible for linalool to undergo acid-catalyzed ring closure to yield mainly alpha-terpineol and minor amounts of the primary terpenoid alcohols, geraniol and nerol. alpha-Linalyl acetate is calculated to have a half-life for hydrolysis of 174 days at pH 8 and 4.7 years at pH 7. Terpineol acetate is calculated to have a half-life for hydrolysis of 2.1 years at pH 8 and 21 years at pH 7. Experimental data indicate a more rapid rate of hydrolysis to yield the component alcohol. The mean half-life for hydrolysis of linalyl acetate at pH 1.2 was less than 2.5 minutes in aqueous artificial gastric juice in the absence or presence of hydrolytic enzymes. When the gastric juice was neutralized to pH 7.0 the half-life increased to 112 minutes. The hydrolysis half-life in aqueous artificial pancreatic fluid in the absence or presence of pancreatin enzyme at pH 7.5 was 97 and 83 minutes, respectively. Ester hydrolysis of linalyl acetate yields linalool and acetic acid. Linalool then partially rearranges to *alpha*-terpineol in both neutral and acidic media. The product ratio of linalool/*alpha*-terpineol was approximately 2: 1 at pH 1.2 or pH 7.5 [Buck and Renwick, 1999]. Mean half-life for alpha-terpineol acetate at pH 1.2 in the absence or presence of hydrolytic enzymes was 18.3 and 16.4 minutes, respectively. When pH was increased to 7.5, the half-life increased to 860 minutes. The hydrolysis half-life of *alpha*-terpineol acetate in aqueous artificial pancreatic fluid in the absence or presence of pancreatin enzyme at pH 7.5 was 358 and 371 minutes, respectively. Based on these data, either ester is anticipated to be completely hydrolyzed to the component acid and alcohol in aqueous media within one day.

3.2.3 Biodegradation

Two separate studies on linalool show this substance is readily biodegradable (*i.e.,* 97.1% biodegradation by OECD 301B and greater than 80% by modified MITI test at 28 days) [Quest, 1994d; Rudio, 1991]. The biodegradabilities of tetrahydrolinalool, myrcenol and dihydromyrcenol have also been measured. Tetrahydrolinalool and dihydromyrcenol were 103% and 72%, degraded, respectively, within 28 days in an OECD 301B assay [Quest, 1994b; Quest 1994c]. Myrcenol was 66% degraded in a 20-day closed bottle assay [UCC, 1986].

Two tertiary terpenoid esters have also been shown to be readily biodegradable. Linalyl acetate underwent 75% biodegradation after 28 days in an OECD modified MITI test [Quest, 1991] and alpha-terpineol acetate exhibited 87.3% and 63% biodegradation in an OECD 301B test [Quest, 1994a] and an OECD 301F test [Givaudan Roure, 1996b], respectively. While no studies are available on *cis*- or *trans*-2-pinanol, there is no reason to believe that these materials will not also be readily biodegradable. The site-restricted chemical intermediate 2-pinanol hydroperoxide will decompose to 2-pinanol [Schmidt and Fisher, 1959] in the environment and thus should be considered to be readily biodegradable. Pliny1 acetate was only 6% degraded in a 28-day OECD 301F test [Mead, 1997b]. This result is inconsistent with the biodegradability results for linalyl acetate and alpha-terpineol acetate in which ultimate biodegradability was observed. In an activated sludge respiration inhibition test the no effect concentration (NOEC) for plinyl acetate was determined to be 100 mg/L [Mead, 1997c]. In an older biodegradability study reporting limited data [Ryckman, 1966], pine oil underwent appreciably biodegradation as measured by a 5-day BOD (0.8 mg/ml) 50% of the measured COD (1.6 mg/ml).

3.2.4 Fugacity

Transport and distribution in the environment were modeled using Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11 [Mackay, 1991]. The principal input parameters into the model are molecular weight, melting point, vapor pressure, water solubility, and log Kow. Where measured values were available, these were used, but where

they were not, calculated data from the EPIWIN series of programs were used. Based on the hydrolysis of the esters to yield component tertiary alcohols and comparable physiochemical properties of the tertiary alcohols, it is not unexpected that the alcohols in this category would exhibit similar distribution in the environment. The distribution of 2-pinanol in the environment is represented by the fugacity calculation for its *cis*- and *trans*-isomers.

The significance of these calculations must be evaluated in the context that the substances in this chemical category are products of plant biosynthesis and are, therefore, ubiquitous in the environment. Most have been shown to be readily and/or ultimately biodegradable, and the remainder would be expected to behave similarly in the environment. The model does not account for the influence of biogenic production on partitioning in the environment nor does it take into account biodegradation. Therefore, the relevance of fugacity calculations for these substances is highly questionable.

3.2.5 New testing required

None

3.3 Ecotoxicity

3.3.1 Acute Toxicity to Fish

Calculated ECOSAR values and nine studies of acute fish toxicity are available for this chemical category. Calculated 96 hr ECOSAR values are in the range from 0.60 mg/L for linalool (calculated as a vinyl alcohol) to 18.2 mg/L for *cis* or *trans*-2-pinanol. With few exceptions, the calculated LC50 values were significantly less than actual experimental values. The 96 hr LC50 values for pine oil in bluegill and rainbow trout in flow-through systems were reported to be 53 and 18 mg/L, respectively [Graves *et al.*, 1994a, 1994b]. In other acute toxicity experiments with pine oil, the 48 hr LC50 value was determined to be 58-59 mg/L for bluegill [Ryckman, 1965] and the 96 hr LC50 value was 71 mg/L in juvenile rainbow trout. The later result was obtained in a range finding study that was used to determine nominal concentrations for a

subsequent 96 hr LC50 flow-through test in the same species [Graves et *al.*, 1994b]. Calculated 96 hr LC50 values for 2-pinanol and *alpha-terpineol*, components of pine oil, are in the same range, 18.2 mg/L and 13.7 mg/L, respectively. An isomer of linalool, isolinalool, exhibited a 96 hr LC50 of 33 mg/L in juvenile rainbow trout [LeLievre, 1990a].

Good correlation exists between the experimental and calculated 96 hr LC50 values for plinyl acetate and myrcenol. The 96 hr LC50 value for rainbow trout exposed to plinyl acetate is reported to be 11.0 mg/L [Wetton, 1997a] while the calculated ECOSAR value is 17.4 mg/L. The measured 96 hr LC50 value for myrcenol in fathead minnows was reported to be 3.7 mg/L [UCC, 1986], which is closely correlated with the calculated 96 hr LC50 of 4.85 mg/L [ECOSAR]. This latter study may be considered of limited value for assessing acute fish toxicity in that minimal aeration was supplied when the dissolved oxygen fell below 4 mg/L.

In a static system test *in* which *alpha-terpineol* was used in conjunction with an emulsifier (10%), the 96 hr LC50s for Coho salmon and rainbow trout were reported to be 6.8 and 6.7 mg/L, respectively [Stroh et *al.*, 1998]. The calculated 96 *hr* LC50 value for *alpha*-terpineol is 13.7 mg/L.

Although there are sufficient data on this chemical category, conducting an assay with linalool following OECD Guideline 203 would provide key data in order to validate the QSAR algorithm and to help determine whether this material should be considered as a vinyl alcohol or as a neutral organic.

3.3.2 Acute Toxicity to Aquatic Invertebrates

In addition to ECOSAR calculated 48 hr LC50 values, experimental data from 4 studies are available for members of this chemical category. Similar to fish acute toxicity data, 48 hr LC50 values are typically lower by an order of magnitude than experimental values. Calculated values are in the range from 4.4 to 20.6 mg/L for tertiary terpenoid alcohols and 1.04 to 1.16 for tertiary terpenoid esters [ECOSAR]. The 48 hr LC50 for myrcenol with *D. magna* was 36 mg/L [UCC, 1986] while the calculated value was 5.75 mg/L. The 48 hr EC50 values with *D.*

magna were reported to be 7.0 mg/L for plinyl acetate [Wetton, 1997b] and 24 mg/L for pine oil [Graves *et al.*, 1994c]. Both studies were performed using OECD 202 guidelines. The value of 24 mg/L for pine oil is in good agreement with the ECOSAR calculated value of 15.7 mg/L for alpha-terpineol, a principal component of pine oil. The reported 48 hr EC50 level for isohnalool *with Daphnia pulex* was reported to be 47 mg/L [LeLievre, 1990b]. Given the available data for members of this chemical category, the approximate range of acute toxicity to aquatic invertebrates, particularly *D. magna,* is expected to be in the range of 10-50 mg/L. Given the low calculated LC50 values for tertiary terpenoid esters, it is recommended that an additional LC50 assay be performed for *D. magna* with linalyl acetate using an OECD 202 Guideline.

3.3.3 Acute Toxicity to Aquatic Plants

In a manner similar to fish and invertebrate toxicity, calculated 96 hr EC50 values for plant *(i.e.,* green algae) are lower than experimental values. Calculated values are in the range from 0.14 to 13.6 mg/L with the majority of values falling in the 3-5 mg/L range for the tertiary alcohols and less than 1 mg/L for tertiary terpenoid esters. Experimental data from 4 studies are available for members of this chemical category and EC50 values are consistently higher than the calculated values. Both linalool and *alpha-terpineol* were subjected to a plate inhibition assay with Chlorella pyrenoidosa using test concentrations of 100, 1000 and 10,000 mg/L [Ikawa *et al.,* 1992]. *alpha-Terpineol* showed no inhibition at any concentration, while linalool showed only mild reduction in colony density as reflected in lawn color at the highest concentration. In a test following OECD 201 Guideline, the reported algal 72 hr EC50 value was greater than 15 mg/L for plinyl acetate in Scenedesmus subspicatus [Mead, 1997a]. A 96 hr NOEC of 3.3 mg/L was reported for isolinalool in Selenastrum capricomutum [Giddings, 1990]. The three measured EC50 values for linalool, *alpha-terpineol,* and plinyl acetate and the single NOEC concentration for isolinalool are all greater than their respective calculated EC50 values. The current database indicates that the EC50 values for members of this chemical category would be in the range of greater than 10-20 mg/L. Given the limited database of information for esters and pinanol

derivatives in this chemical category, it is recommended that acute EC50 assays be performed for linalyl acetate and 2-pinanol using OECD Guideline 20 1.

3.3.4 New Testing Required

Acute toxicity to fish by OECD guideline 203 for linalool;

Acute toxicity to aquatic invertebrates by OECD guideline 202 for linalyl acetate;

Acute toxicity to aquatic plants by OECD Guideline 201 for linalyl acetate and 2-pinanol.

3.4 Human Health Data

3.4.1 Acute Toxicity

Oral and dermal LD50 values for members of this chemical category indicate a low order of both oral and dermal toxicity. All rabbit dermal, and mouse and rat oral LD50 values exceed 2000 mg/kg with the majority of values greater than 5000 mg/kg [Baker et al., 1976; Cerven, 1985a, 1985b; Deichmann, 1961; Jenner, 1964; Johnson, 1976; Moreno, 1972a, 1972b, 1973, 1976; Palanker, 1979; Robbins, 1994; Sanders, 1997, Fogelman, 1970].

3.4.2 *In* vitro Genotoxicity

Mutagenicity/genotoxicity testing has been performed on six members of this chemical category, including a complete battery of *in vitro* genotoxicity tests using linalool. Linalool [Heck *et al.,* 1989, Ishidate *et al.,* 1984; Florin *et al.,* 1980; Rockwell and Raw, 1979] and tetrahydrolinalool [Wild *et al.,* 1983] were inactive *in Salmonella typhimurium (SAL) strains* TA92, TA94, TA98, TA100, TA1535, TA1537, and TA1538 with and without S-9 metabolic activation. Linalool did not induce chromosomal aberrations when incubated with Chinese hamster fibroblast cells at a maximum concentration of 0.25 mg/ml [Ishidate *et al.,* 1984], nor did it induce unscheduled DNA synthesis (UDS) in rat hepatocytes at concentrations up to 50 nl/ml [Heck *et al.*, 1989].

When incubated with *E. coli WP2 uvrA* at concentrations of 125- 1000 mg/plate, linalool was negative for mutation induction [Yoo, 1986]. When incubated with *Bacillus subtilis* H 17 (rec+) and M45 (rec-), linalool was negative at 17 µg [Oda *et al.,* 1978] but positive at 10 µl/disk

[Yoo, 1986]. The latter result occurred in a study in which the majority of alcohols and aldehydes were positive while non-oxidizable substrates (esters, ketones, lactone, and acid) were negative. The positive responses in that study [Yoo, 1986] are clearly contradicted by the results of the same assay by other researchers [Oda *et al.,* 1978]. In a mouse lymphoma assay, linalool was negative in L5 178Y TK+/- cells with S-9 metabolic activation at 200 nl/ml but weakly positive without S-9 activation at 150 nl/ml [Heck *et al.,* 1989].

Linalyl acetate and *alpha-terpineol were inactive in Salmonella typhimurium (SAL) strains* TA98, TAlOO, TA1535, TA1537, and TA1538 with and without S-9 metabolic activation [Heck et *al.,* 1989; Ishidate *et al.,* 1984; Florin *et al.,* 1980]. *p*-Menth-8-en-1-ol (*alpha*-terpineol) was inactive in SAL strains TA98 and TAlOO with S-9 metabolic activation [Rockwell and Raw, 1979]. When incubated with *Bacillus subtilis* H17 (rec+) and M45 (rec-), hnalyl acetate and terpinyl acetate were negative at 18 µg and 19 µg, respectively [Oda *et al.,* 1978].

In an *in vivo-in vitro* study designed to investigate the mutagenicity of the metabolites of linalool and alpha-terpineol, Sprague-Dawley rats were administered a single dose of 0.5 ml (452 mg) of linalool or alpha-terpineol by gavage and the urine was collected for 24-hours. The urine (500 ul) was hydrolyzed *with beta-glucuronidase.* Hydrolyzed and unhydrolyzed urine samples, ether extracts of the urine, and aqueous fractions of the urine-ether extracts were then separately incubated with SAL strains TA98 and TAlOO without S9 activation. Linalool, *alpha*-terpineol, and none of the urinary solutions isolated from the urine of rats given 452 mg doses of either linalool or *alpha-terpineol* showed any evidence of mutagenicity in either TA98 or TAlOO without metabolic activation [Rockwell and Raw, 1979].

In nineteen separate *in vitro* tests on the mutagenicity and genotoxicity of terpenoid tertiary alcohols and related esters, all but two were negative. One of the positive results for linalool was observed in a rec assay using differences in growth rates *in two strains* of *Bacillus subtilis* as a measure of DNA changes [Yoo, 1986]. In contrast, no evidence of mutagenicity was observed in the same test at a higher concentrations [Oda *et al.,* 1978] nor was DNA damage observed

in a rat hepatocyte UDS assay [Heck et *al.,* 1989]. The authors of the mouse lymphoma assay [Heck et *al.,* 1989], which gave a weak positive result for linalool, emphasized that positive results in this assay are commonly observed for polar substances in the absence of S-9 and may be associated with changes in physiologic culture conditions (pH and osmolality).

3.4.3 *In* vivo Genotoxicity

In a standardized mouse micronucleus assay, male and female CD- 1 mice were given single intraperitoneal injections of 116, 578, or 1155 mg/kg pine oil and bone marrow samples were retrieved at 24, 48, and 72 hours. There was no evidence of an increased incidence of micronucleated polychromatic erythrocytes at any dose level tested [Putman, 1987].

Based on a weight of evidence evaluation of the available in *vitro* and *in vivo* mutagenicity and genotoxicity assays on terpenoid tertiary alcohols and related esters, this group of flavoring substances would not be expected to exhibit a low genotoxic potential *in vivo.*

3.4.4 Repeat Dose Toxicity

3.4.4.1 Linalool

In a safety evaluation study, a 50/50 mixture of linalool and citronellol was fed to male and female rats (number and strain not specified) in the diet. The daily intake was calculated to be 50 mg/kg bw of each. Measurements of hematology, clinical chemistry, and urinalysis at weeks 6 and 12 showed no statistically significant differences between test and control groups. Histopathology revealed no dose-related lesions. A slight retardation of growth was observed in males only, but was concluded by the authors to be biologically insignificant [Food and Drug Research Lab., 1958].

3.4.4.2 Linalyl esters

For 12 weeks, a mixture of linalyl acetate, linalyl isobutyrate and geranyl acetate was added to the diet of male and female rats (strain not specified) at levels calculated to result in average daily intakes of 24, 27, or 48 mg/kg bw, respectively. Measurements of hematology, clinical

chemistry, and urinalysis at weeks 6 and 12 showed normal values. Histopathology revealed no dose-related lesions. A slight retardation of growth was observed in females only, but was concluded by the authors to be biologically insignificant [Trubeck Laboratories, 195 8].

Four groups of 10 male and 10 female Osborne-Mendel rats were fed the structurally related ester of linalool, linalyl isobutyrate, at dietary concentrations of 0, 1000, 2500, or 10,000 ppm for 18 weeks. These levels were calculated [FDA, 1993] to provide estimated daily intakes of 0, 50, 125, or 500 mg/kg bw, respectively. Body weight, hematology, and gross pathology were performed on all test animals, and microscopic examination was performed on the high dose group only. There were no differences between treated and control animals in the parameters evaluated [Hagan et al., 1967].

In a co-carcinogenicity study, 3 mg of linalyl acetate was applied either alone or in conjunction with the carcinogen benzo-[a]-pyrene to the skin of female ICR/Swiss Ha mice (20/group) 3 times per week for 67 weeks. Mice showing tumors for 30 days or more, greater than 1 mm in size, were counted. There was no increase in the incidence of tumors in mice treated with linalyl acetate itself or with benzo-[a]-pyrene [Van Duuren *et al.,* 1971].

3.4.4.3 alpha-Terpineol acetate

Ten (10) male and 10 female weanling Osborne-Mendel rats were fed terpinyl acetate in the diet for 20 weeks at concentrations of 0, 1000, 2500 or 10,000 ppm [Hagan *et al.,* 1967]. These dietary levels were calculated [FDA, 1993] to result in daily intakes of 0, 50, 125 and 500 mgikg bw, respectively. All animals were examined for growth, hematology, and macroscopic changes in the tissues. Microscopic examination was performed on 6-8 male and female animals in the high dose and control groups. No statistically significant adverse effects were reported [Hagan *et al.,* 1967].

3.4.4.4 2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate)

Following a range- finding, repeat-dose toxicity study [Thomas, 1997], groups of male and female Sprague-Dawley rats were administered 0, 15, 150,0r 1000 mg/kg/d of plinyl acetate by gavage daily for 28 days. Based on the results of daily observation for clinical signs, weekly measurement of body weight and food consumption, hematologkal examinations, blood chemical determinations, measurement of organ weights and gross and histopathological examination, it was concluded that 15 mg/kg/d was a NOAEL for plinyl acetate in male and female rats. At the 150 mg/kg/d level, a statistically significant increase in liver and kidney weights was accompanied by histopathological changes including accumulation of globular eosinophilic material in male kidney, and centrilobular hepatocyte enlargement in male rats [Thomas, 1997].

3.4.5 Reproductive Toxicity

Four groups of 10 virgin Crl CD rats were administered 0, 250, 500, or 1000 mg/kg bw of an essential oil (coriander oil) known to contain 73% linalool by mass. The test material was given by gavage once daily, 7 days prior to cohabitation, through cohabitation (maximum of 7 days), gestation, delivery, and a 4-day post-parturition period. The duration of the study was 39 days. Maternal indices monitored included twice daily observation, measurement of body weights, food consumption, duration of gestation, and fertility parameters (mating and fertility index, gestation index, number of offspring per litter). Offspring indices included daily observation, clinical signs, examination for gross external malformations, and measurement of body weight. Maternal effects reported included increased body weight and increased food consumption at 250 mg/kg/d, a non-statistically significant decrease in body weight and food consumption and decreased gestation index and decreased length of gestation at 500 mg/kg/d, and a statistically significant decrease in body weight and food consumption, statistically significant decrease in gestation index, length of gestation, and litter size at 1000 mg/kg/d. The only effect on pups was a decrease in viability of pups at the highest dose level. The authors concluded that there were no effects observed in the dams at the low dose of 250 mg/kg bw/d or in the offspring at the

250 and 500 mg/kg bw/d levels. The authors concluded that the maternal NOAEL was 250 mg/kg/d and the developmental NOAEL was 500 mg/kg/d [Vollmuth *et al.*, 1995].

Four groups of 10 virgin Crl CD rats were administered 0, 375, 750, or 1500 mg/kg bw of an essential oil (cardamom oil) known to contain greater than 65 % tertiary terpenoid alcohols with 5 1% alpha-terpineol acetate by mass. The test material was given by gavage once daily, 7 days prior to cohabitation, through cohabitation (maximum of 7 days), gestation, delivery, and a 4-day post-parturition period. The duration of the study was 39 days. Maternal indices monitored included twice-daily observation, measurement of body weights, food consumption, duration of gestation, and fertility parameters (mating and fertility index, gestation index, number of offspring per litter). Offspring indices included daily observation, clinical signs, examination for gross external malformations, and measurement of body weight. Maternal observations included a non-statistically significant decrease in body weight gain and food consumption at 375 mg/kg/d. Mortality, clinical signs, a statistically significant decrease in body weight gain and food consumption, and gross lesions at necropsy were seen at 750 and 1500 mg/kg/d. The only effects on pups were a reduced body weight gain in pups at 750 and 1500 mg/kg/d and increased mortality at 1500 mg/kg/d. The authors concluded that there were no significant adverse effects in the dams or offspring at the 375 mg/kg/d dose. A maternal NOEL was reported to be less than 375 mg/kg/d based on reduced body weight gain and food consumption at 375 mg/kg/d and a developmental NOAEL was reported to be 375 mg/kg/d [Vollmuth *et al.*, 1995].

3.4.6 Developmental/Teratogenicity Toxicity

In addition to the two developmental/reproduction screening studies above, a range-finding study and follow-up teratology study was performed with pine oil. Pregnant Crl:CD(SD) BR rats were given 0, 50, 100, 500, 750,or 1000 mg/kg/d by gavage in corn oil on days 6 to 20 of gestation. Laparotomies were performed, corpora lutea were counted, and the uterus of each rat was removed, weighed and then examined for number, placement and viability of implantations. Live fetuses were weighed, sexed and gross external alternations were identified.

Soft tissue and skeletal evaluations were not performed in the pilot study. There were no deaths or abortions during the course of this study. Necropsy revealed no gross lesions. Maternal effects included local alopecia, decreased body weight gain and food consumption for the 3 highest dose levels. At 750 and 1000 mg/kg, average gravid uterine weight was reduced. In fetuses, decreased body weight was observed at dose levels of 100 mg/kg and above, and at dose levels of 500 and above there was a slight increase in average number of resorptions/litter [Dearlove, 1987].

In the follow-up teratology study, pregnant Crl:CD(SD) BR rats were given 0, 50, 600, or 1200 mg/kg/d by gavage in corn oil on days 6 to 20 of gestation. Rats were examined for pregnancy, number and placement of implantations, early and late resorptions, live and dead fetuses, and number of corpora lutea. Fetuses were subsequently weighed and evaluated for both soft and hard tissue abnormalities. At 600 and 1200 mg/kg/d, decreased food consumption, body weight gains, excess salivation, alopecia, ungroomed coat, ataxia, decreased motor activity, impaired righting reflex and urine stained abdominal fur were observed Six of the 25 rats in 1200 mg/kg dose group died and necropsies revealed that adrenal weights were significantly increased in these rats. At 1200 mg/kg/d, fetuses exhibited increased incidences of delayed ossification, delayed brain development, decreased weights, increased embryo -fetal mortality, and sunken eye bulge with associated soft and hard tissue findings, a dose that also resulted in maternal death and a low incidence of embryo-fetal death (resorption). The maternal and developmental NOEL for pine oil was greater than 50 mg/kg/d but less than 600 mg/kg/d [Parent, 1988].

3.4.7 New Testing Required

None

3.5 Test Plan Table

Chemical	Physical-Chemical Properties				
	Melting Point	Boiling Point	Vapor Pressure	Partition Coefficient	Water Solubility
CAS No. 78-70-6 Linalool (3,7-dimethyl-1,6-octadien-3-ol)	A	A, Calc	A, Calc	A, Calc	A, Calc
CAS No. 78-69-3 Tetrahydrolinalool (3,7-Dimethyl-3-Octanol)	Calc	A	Calc	Calc	A, Calc
CAS No. 543-39-5 Myrcenol (2-methyl-6-methylene-7-octen-2-ol)	Calc	A	Calc	Calc	Calc
CAS No. 18497-58-8 Dihydromyrcenol (3,7-dimethyl-7-octen-2-01)	Calc	A, Calc	Calc	Calc	Calc
CAS No. 115-95-7 Linalyl acetate (3,7-dimethyl-1,6-octadien-3-yl acetate	Calc	A, Calc	Calc	A, Calc	A, Calc
CAS No.98-55-5 alpha-Terpineol (p-menth-1-en-8-	Calc	A	A, Calc	A, Calc	A, Calc
CAS No. 80-26-2 alpha-Terpinyl acetate (p-menth-1-en-8-yl acetate)	Calc	A	Calc	A, Calc	Calc
CAS No. 125252-49-5 2,6,6-Trimethylbicyclo[3.1.1]heptan-2-01 thermal rearrangement products	NA	A	A	A, Calc	A, Calc
CAS No. 4948-28-l *cis*-2-Pinanol	NA	A, Calc	Calc	Calc	Calc
CAS No 473-54-l Pinanol	Calc	A	Calc	Calc	R
CAS No. 4948-29-2 trans-2-Pinanol	NA	A, Calc	Calc	Calc	R
CAS No. 28324-52-9 2-Pinanol hydroperoxide	NA	NA	NA	Calc	Calc
CAS No. 8002-09-3 Pine oil	NA	A	Calc	Calc	A

Chemical	Environmental Fate and Pathways			
	Photodegra-dation	Stability in Water	Biodegra-dation	Fugacity
CAS No. 78-70-6 Linalool (3,7-dimethyl-1,6-octadien-3-ol)	Calc	A	A	Calc
CAS No. 78-69-3 Tetrahydrolinalool (3,7-Dimethyl-3-Octanol)	Calc	NA	A	Calc
CAS No. 543-39-5 Myrcenol (2-methyl-6-methylene-7-octen-2-ol)	Calc	NA	R	Calc
CAS No. 18497-58-8 Dihydromyrcenol (3,7-dimethyl-7-octen-2-ol)	Calc	NA	A	Calc
CAS No. 115-95-7 Linalyl acetate (3,7-dimethyl-1,6-octadien-3-yl acetate	Calc	A	A	Calc
CAS No.98-55-5 alpha-Terpineol (p-menth-l-en-%01)	Calc	NA	R	Calc
CAS No. 80-26-2 alpha-Terpinyl acetate (p-menth-1-en-8-yl acetate)	Calc	A	A	Calc
CAS No. 125252-49-5 2,6,6-Trimethylbicyclo[3.1.1]heptan-2-01 thermal rearrangement products	R	NA	A	Calc
CAS No. 4948-28-l cis-2-Pinanol	Calc	NA	R	Calc
CAS No 473-54-l Pinanol	R	NA	R	R
CAS No. 4948-29-2 *trans*-2-Pinanol	R	NA	R	Calc
CAS No. 28324-52-9 2-Pinanol hydroperoxide	Calc	NA	R	Calc
CAS No. 8002-09-3 Pine oil	R	NA	A	Calc

Chemical	Ecotoxicity		
	Acute Toxicity to Fish	Acute Toxicity to Aquatic Invertebrates	Acute Toxicity to Aquatic Plants
CAS No. 78-70-6 Linalool (3,7-dimethyl-1,6-octadien-3-ol)	R,Calc, T	R	A. Calc
CAS No. 78-69-3 Tetrahydrolinalool (3,7-Dimethyl-3-Octanol)	R, Calc	R, Calc	R, Calc
CAS No. 543-39-5 Myrcenol (2-methyl-6-methylene-7-octen-2-ol)	A, Calc	A, Calc	R, Calc
CAS No. 18497-58-8 Dihydromyrcenol (3,7-dimethyl-7-octen-2-ol)	R, Calc	R, Calc	R, Calc
CAS No. 115-95-7 Linalyl acetate (3,7-dimethyl-1,6-octadien-3-yl acetate	R, Calc	T, Calc	T, Calc
CAS No.98-55-5 alpha-Terpineol (p-menth-1-en-8-01)	A, Calc	R, Calc	A, Calc
CAS No. 80-26-2 alpha-Terpinyl acetate (p-menth-1-en-8-yl acetate)	R, Calc	R, Calc	R, Calc
CAS No. 125252-49-5 2,6,6-Trimethylbicyclo[3.1.1]heptan-2-01 thermal rearrangement products	A, Calc	A	A
CAS No. 4948-28-l cis-2-Pinanol	R, Calc	R, Calc	R, Calc
CAS No 473-54-l 2-Pinanol	R	R	T
CAS No. 4948-29-2 *trans*-2-Pinanol	R, Calc	R	R
CAS No. 28324-52-9 2-Pinanol hydroperoxide	R, Calc	R, Calc	R
CAS No. 8002-09-3 Pine oil	A, Calc	A	R

Chemical	Human Health Data					
	Acute Toxicity	Genetic Toxicity *In Vitro*	Genetic Toxicity *In Vivo*	Repeat Dose Toxicity	Repro-ductive Toxicity	Develop-mental Toxicity
CAS No. 78-70-6 Linalool (3,7-dimethyl-1,6-octadien-3-ol)	A	A	R	A	A	R
CAS No. 78-69-3 Tetrahydrolinalool (3,7-Dimethyl-3-Octanol)	A	A	R	R	R	R
CAS No. 543-39-S Myrcenol (2-methyl-6-methylene-7-octen-2-ol)	A	R	R	R	R	R
CAS No. 18497-58-8 Dihydromyrcenol (3,7-dimethyl-7-octen-2-ol)	A	R	R	R	R	R
CAS No. 115-95-7 Linalyl acetate (3,7-dimethyl-1,6-octadien-3-yl acetate	A	A	R	A	R	R
CAS No.98-55-5 alpha-Terpineol (p-menth-1-en-S-01)	A	A	R	R	R	R
CAS No. 80-26-2 *alpha*-Terpinyl acetate (p-menth-1-en-8-yl acetate)	A	A	R	A	A	R
CAS No. 125252-49-s 2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products	A	A	R	A	R	R
CAS No. 4948-28-l *cis*-2-Pinanol	A	R	R	R	R	R
CAS No 473-54-l Pinanol	R	R	R	R	R	R
CAS No. 4948-29-2 *trans*-2-Pinanol	R	R	R	R	R	R
CAS No. 28324-52-9 2-Pinanol hydroperoxide	R	R	R	R	R	R
CAS No. 8002-09-3 Pine oil	A	A	A	R	R	A

Legend	
Symbol	**Description**
R	Endpoint requirement fulfilled using category approach, SAR
T	Endpoint requirements to be fulfilled with testing
Calc	Endpoint requirement fulfilled based on calculated data
A	Endpoint requirement fulfilled with adequate existing data
NR	Not required per the OECD SIDS guidance
NA	Not applicable due to physical/chemical properties
0	Other

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The Flavor and Fragrance High Production Volume Consortia

Robust Summaries for Terpenoid Tertiary Alcohols and Related Esters

FFHPVC Terpene Consortium Registration Number

The evaluation of the quality of the following data uses a systematic approach described by Klimisch [Klimisch et al., 1996]. Based on criteria relating to international testing standards for categorizing data reliability, four reliability categories have been established. The following categories are:

- Reliability code 1. Reliable without restrictions
- Reliability code 2. Reliable with restrictions
- Reliability code 3. Not reliable
- Reliability code 4. Not assignable

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1 Chemical and Physical Properties

1.1 Melting Point

Substance Name	Linalool (3,7-Dimethyl-1 ,6-octadien-1-ol)
CAS No.	**78-70-6**
Method/guideline	Not specified
Melting Point	<20 °C
Conclusion Remarks	Consistent with calculated weighted MP determination (SRC)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Givaudan Roure (1991a) Determination of ready biodegradability of linalool. Unpublished report.

Substance Name	Tetrahydrolinalool
CAS No.	**78-69-3**
Method/guideline	Mean or weighted MP
Melting Point	-11.8 °C
Conclusion Remarks	Calculated melting point

Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Syracuse Research Corporation (SRC)

Substance Name	Myrcenol
CAS No.	**543-39-5**
Method/guideline	Mean or weighted MP
Melting Point	-13.4 °C
Conclusion Remarks	Calculated melting point
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Syracuse Research Corporation (SRC)

Substance Name	Dihydromyrcenol
CAS No.	18479-58-8
Method/guideline	Mean or weighted MP
Melting Point	-13.4 °C
Conclusion Remarks	Calculated melting point
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Syracuse Research Corporation (SRC)

Substance Name	Linalyl acetate
CAS No.	115-95-7
Method/guideline	Mean or weighted MP
Melting Point	-2.1 °C
Conclusion Remarks	Calculated melting point
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Syracuse Research Corporation (SRC)

Substance Name	alpha-Terpineol
CAS No.	98-55-5

Method/guideline	Mean or weighted MP
Melting Point	12.4 °C
Conclusion Remarks	Calculated melting point, measured solidification temperature for *l* isomer = 36.4 °C and *d* isomer 31 .O °C (Merck, 1997)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Syracuse Research Corporation (SRC)

Substance Name	alpha-Terpinyl acetate
CAS No.	80-26-2
Method/guideline	Mean or weighted MP
Melting Point	21.4 °C
Conclusion Remarks	Calculated melting point
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Syracuse Research Corporation (SRC)

Substance Name	2-Pinanol
CAS No.	473-54-l
Method/guideline	Mean or weighted MP
Melting Point	**22.9** °C
Conclusion Remarks	Calculated melting point
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Syracuse Research Corporation (SRC)

1.2 Boiling Point

Substance Name	cis-2-Pinanol
CAS No.	4948-28-l
Boiling Point	205 °C
Pressure	760

Pressure Unit	mm Hg
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Fragrance Materials Association (FMA)

Substance Name	2-Pinanol
CAS No.	473-54-l
Boiling Point	205 °C
Pressure	760
Pressure Unit	mm Hg
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Fragrance Materials Association (FMA)

Substance Name	*trans*-2-Pinanol
CAS No.	**4948-29-2**
Boiling Point	205206 °C
Pressure	760
Pressure Unit	mm Hg
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Fragrance Materials Association (FMA)

Substance Name	Pine oil
CAS No.	**8002-09-3**
Boiling Point	200-220 °C
Pressure	760
Pressure Unit	mm Hg
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Fragrance Materials Association (FMA)

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)

CAS No.	**125252-49-5**
Method/guideline	Using differential scanning calorimetry, ASTM E 537-86 and Method A2 of Commission Directive 92/69/EEC
GLP	Yes
Year	1997
Boiling Point	492 +/- 0.5K (219 “C)
Pressure	101.82
Pressure Unit	kPa
Remarks for Results	Boiling Temperature: 492 +/- 0.5 K
Conclusion Remarks	The boiling temperature of plinyl acetate was determined to be 492 +I- 0.5K at a pressure of 101.82 kPa.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Reliabilities	The study was performed in compliance with the UK GLP and these Principles are in accordance with GPL standard published as OECD Environment Monograph No. 45 (OCDE/GD(92)32).
References	Lumsden A. M. (1998) Plinyl Acetate: Determination of general physico-chemical properties. Safepharm Laboratories, Inc. SPL Project Number: 1044/001.

Substance Name	Myrcenol
CAS No.	**543-39-5**
Boiling Point	**213** °C
Pressure	**760**
Pressure Unit	mm Hg
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Fragrance Materials Association (FMA)

Substance Name	Dihydromyrcenol
CAS No.	**18479-58-8**
Boiling Point	**80** °C
Pressure	**213**
Pressure Unit	mm Hg
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Fragrance Materials Association (FMA)

Substance Name	Linalool
CAS No.	**78-70-6**
Boiling Point	**198 °C**
Pressure	**760**
Pressure Unit	mm Hg
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Fragrance Materials Association (FMA)

Substance Name	Linalool
CAS No.	**78-70-6**
Boiling Point	**198 °C**
Pressure	**760**
Pressure Unit	mm Hg
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Food and Agricultural Organization of the United States (FAO) (1997) Compendium of food additive specifications addendum 5.

Substance Name	Linalyl acetate
CAS No.	**115-95-7**
Boiling Point	213 °C
Pressure	760
Pressure Unit	mm Hg
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
References	Fragrance Materials Association (FMA)

Substance Name	Tetrahydrolinalool
CAS No.	78-69-3
Boiling Point	230°C
Pressure	760

Pressure Unit	mm Hg
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions,
References	Fragrance Materials Association (FMA)

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Boiling Point	218 °C
Pressure	760
Pressure Unit	mm Hg
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Fragrance Materials Association (FMA)

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Boiling Point	206-207 °C
Pressure	731
Pressure Unit	mm Hg
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Merck Index (1997) Merck & Co., Inc. Publishers: Merck Research Laboratories, 12th edition, Whitehouse Station, NJ.

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Boiling Point	217 °C
Pressure	760
Pressure Unit	mm Hg
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Food and Agricultural Organization of the US (FAO) (1997) Compendium of food additive specifications addendum 5.

Substance Name	alpha-Terpinyl acetate

CAS No.	**80-26-2**
Boiling Point	**220 °C**
Pressure	**760**
Pressure Unit	mm Hg
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Food and Agricultural Organization of the US (FAO) (1997) Compendium of food additive specifications addendum 5.

Substance Name	alpha-Terpinyl acetate
CAS No.	**80-26-2**
Boiling Point	**220 °C**
Pressure	**760**
Pressure Unit	mm Hg
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Merck Index (1997) Merck & Co., Inc. Publishers: Merck Research Laboratories, 12th edition, Whitehouse Station, NJ.

Substance Name	2,6,6-Trimethylbicyclo[3. 1. 1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)
CAS No.	**125252-49-5**
Boiling Point	**196 °C**
Pressure	**760**
Pressure Unit	mm Hg
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Lumsden A. M. (1998) Plinyl Acetate: Determination of general physico-chemical properties. Safepharm Laboratories, Inc. SPL Project Number: 1044/001.

Substance Name	Linalool
CAS No.	**78-70-6**
Boiling Point	**198 °C**
Pressure	**760**
Pressure Unit	mm Hg

Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Merck Index (1997) Merck & Co., Inc. Publishers: Merck Research Laboratories, 12th edition, Whitehouse Station, NJ.

Substance Name	Linalool
CAS No.	78-70-6
Method/guideline	Stein and Brown Method
Boiling Point	204 °C
Pressure	760
Pressure Unit	mm Hg
Conclusion Remarks	Calculated
References	Syracuse Research Corporation (SRC)

Substance Name	Dihydromyrcenol
CAS No.	18479-58-8
Method/guideline	Stein and Brown Method
Boiling Point	191 °C
Pressure	760
Pressure Unit	mm Hg
Conclusion Remarks	Calculated
References	Syracuse Research Corporation (SRC)

Substance Name	Linalyl acetate
CAS No.	115-95-7
Method/guideline	Stein and Brown Method
Boiling Point	229 °C
Pressure	760
Pressure Unit	mm Hg
Conclusion Remarks	Calculated
References	Syracuse Research Corporation (SRC)

Substance Name	cis-2-Pinanol
CAS No.	**4948-28-l**
Method/guideline	Stein and Brown Method
Boiling Point	**200.8 °C**
Pressure	**760**
Pressure Unit	mm Hg
Conclusion Remarks	Calculated
References	Syracuse Research Corporation (SRC)

Substance Name	*trans-2-*Pinanol
CAS No.	**4948-29-2**
Method/guideline	Stein and Brown Method
Boiling Point	214 °C
Pressure	760
Pressure Unit	mm Hg
Conclusion Remarks	Calculated
References	Syracuse Research Corporation (SRC)

1.3 Vapor Pressure

Substance Name	alpha-Terpinyl acetate
CAS No.	80-26-2
Method/guideline	Calculated
Vapor Pressure	0.07 mm Hg
Temperature	20 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions,
References	Fragrance Materials Association (FMA)

Substance Name	cis-2-Pinanol
CAS No.	**4948-28-I**
Method/guideline	Calculated
Vapor Pressure	0.05 mm Hg
Temperature	**20 °C**
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Fragrance Materials Association (FMA)

Substance Name	2-Pinanol
CAS No.	473-54-I
Method/guideline	Calculated
Vapor Pressure	0.05 mm Hg
Temperature	20 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Fragrance Materials Association (FMA)

Substance Name	*trans*-2-Pinanol
CAS No.	**4948-29-2**
Method/guideline	Calculated
Vapor Pressure	0.05 mm Hg
Temperature	20 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Fragrance Materials Association (FMA)

Substance Name	Pine oil
CAS No.	**8002-09-3**
Method/guideline	Calculated
Vapor Pressure	0.07 mm Hg

Temperature	20 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Fragrance Materials Association (FMA)

Substance Name	2,6,6-Trimethylbicyclo[3.1 .1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)
CAS No.	**125252-49-5**
Method/guideline	Testing was conducted according to method A4 specified in Commission Directive 92/69/EEC (which constitutes Annex V of Council Directive 67/548/EEC).
Remarks for Test Conditions	The vapor pressure was determined using an isoteniscope system in which sample's vapor pressure was measured using mercury in a glass manometer. The temperature of the sample was regulated by use of a silicone oil bath.
Vapor Pressure	108 Pa = 0.81 mm Hg
Temperature	25 °C
Conclusion Remarks	The vapor pressure was determined to be 108 Pa at 25 C.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The study was performed in compliance with the UK Principles of GLP and these principles are in accordance with GLP standards published as OECD Environment Monograph No. 45 (OECD/GD(92)32).
General Remarks	The vapor pressure was measured over a range of temperature to enable extrapolation to 298.15 K
References	Tremain S. P. (1997). Plinyl Acetate: Determination of Vapor Pressure. Safepharm Laboratories Ltd. SPL Project No. 1044/003.

Substance Name	Myrcenol
CAS No.	**543-39-5**
Method/guideline	Calculated
Vapor Pressure	0.05 mm Hg
Temperature	20 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Fragrance Materials Association (FMA)

Substance Name	Dihydromyrcenol

CAS No.	**18479-58-8**
Method/guideline	Calculated
Vapor Pressure	0.12 mm Hg
Temperature	20 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Fragrance Materials Association (FMA)

Substance Name	Linalool
CAS No.	78-70-6
Method/guideline	Calculated
Vapor Pressure	0.08 mm Hg
Temperature	20 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Fragrance Materials Association (FMA)

Substance Name	Linalool
CAS No.	78-70-6
Method/guideline	Measured
Vapor Pressure	0.05027 mm Hg
Temperature	20 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Vuilleumeier C., Flament I. and P. Sauvegrain (1995) Headspace analysis study of evaporation rate of perfume ingredients applied onto skin. International Journal of Cosmetic Science, 17(1), 61-76.

Substance Name	Linalool
CAS No.	78-70-6
Method/guideline	Measured
Vapor Pressure	0.15 mm Hg
Temperature	20 °C

Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Givaudan Roure (1991a) Determination of ready biodegradability of linalool. Unpublished report.

Substance Name	Linalyl acetate
CAS No.	115-95-7
Method/guideline	Calculated
Vapor Pressure	**0.07** mm Hg
Temperature	**20** °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Fragrance Materials Association (FMA)

Substance Name	Tetrahydrolinalool
CAS No.	**78-69-3**
Method/guideline	Calculated
Vapor Pressure	**0.04** mm Hg
Temperature	**20** °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Fragrance Materials Association (FMA)

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Method/guideline	Calculated
Vapor Pressure	**0.02** mm Hg
Temperature	**20** °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Fragrance Materials Association (FMA)

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**

Year	1995
Vapor Pressure	**0.04** mm Hg
Temperature	**22-25** °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Misra G., Pavlostathis S.G., Li J., and Perdue E. M. (1995) Characterization and Biodegradation of Selected Monoterpenes. 68th Annual Conference & Exposition, Water Environment Federation; Miami Beach, FL.

Substance Name	Linalool
CAS No.	78-70-6
GLP	NA
Year	**1995**
Vapor Pressure	0.16 mm Hg
Temperature	22-25 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Misra G., Pavlostathis S.G., Li J., and Perdue E. M. (1995) Characterization and Biodegradation of Selected Monoterpenes. 68th Annual Conference & Exposition, Water Environment Federation; Miami Beach, FL.

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (data for component alcohol - plinol, clear colorless non-viscous liquid)
CAS No.	125252-49-5
GLP	NA
Year	1995
Vapor Pressure	0.14 mm Hg
Temperature	22-25 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Misra G., Pavlostathis S.G., Li J., and Perdue E. M. (1995) Characterization and Biodegradation of Selected Monoterpenes. 68th Annual Conference & Exposition, Water Environment Federation; Miami Beach, FL.

1.4 Octanol/Water Partition Coefficients

Substance Name	2,6,6-Trimethylbicyclo[3.1 .1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)
CAS No.	**125252-49-5**
Method/guideline	The determination was carried out using the HPLC method, Method A8 of Commission Directive 92/69/EEC (which constitutes Annex V of Council Directive 67/548/EEC).
GLP	Yes
Year	1997
Remarks for Test Conditions	A preliminary assessment of the partition coefficient was made based on the approximate solubilities of the test material in n-octanol and water. This was performed by visual assessment.
Log Pow	4.09
Temperature	21.5 °C
Conclusion Remarks	The partition coefficient of Plinyl acetate was determined to be 1.23X10E4, Log10 Pow = 4.09
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The study was performed in compliance with the UK GLP and these Principles are in accordance with GLP standards published as OECD Environment Monograph No. 45 (OECD/GD(92)/32).
General Remarks	Substance having a log10 Pow of greater than 3 are regard as having the potential of bioaccumulation in the environment.
References	Lumsden A. M. (1998) Plinyl Acetate: Determination of general physico-chemical properties. Safepharm Laboratories, Inc. SPL Project Number: 1044/001.

Substance Name	Myrcenol
CAS No.	**543-39-5**
Method/guideline	Calculated
Log Pow	3.46
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Syracuse Research Corporation (SRC)

Substance Name	Dihydromyrcenol
CAS No.	**18479-58-8**

Method/guideline	Calculated
Log Pow	**3.47**
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Syracuse Research Corporation (SRC)

Substance Name	Linalool
CAS No.	78-70-6
Method/guideline	Calculated
Log **Pow**	3.38
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions,
References	Syracuse Research Corporation (SRC)

Substance Name	Linalool
CAS No.	78-70-6
Method/guideline	Measured Rp-TLC
Log Pow	**2.9**
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Givaudan Roure (1991 b) Determination of the partition coefficient (octanol/water) of linalool. Unpublished report.

Substance Name	Linalyl acetate
CAS No.	115-95-7
Method/guideline	Calculated
Log **Pow**	3.46
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Syracuse Research Corporation (SRC)

Substance Name	Linalyl acetate
CAS No.	**115-95-7**
Method/guideline	Measured

Log Pow	**2.9**
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Proctor & Gamble (1996) Submission to EPA. Unpublished report.

Substance Name	Tetrahydrolinalool
CAS No.	**78-69-3**
Method/guideline	Calculated
Log Pow	**3.6**
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Syracuse Research Corporation (SRC)

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Method/guideline	Calculated
Log Pow	**3.33**
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Syracuse Research Corporation (SRC)

Substance Name	alpha-Terpineol acetate
CAS No.	**80-26-2**
Method/guideline	Measured RP-TLC
Log Pow	**4.3**
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Reference	Givaudan Roure (1996a) Partition coefficient n-octanol/water of alpha-terpineol acetate. Unpublished report.

Substance Name	alpha-Terpineol acetate
CAS No.	**80-26-2**
Method/guideline	Calculated

Log Pow	**4.34**
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Syracuse Research Corporation (SRC)

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)
CAS No.	125252-49-5
Method/guideline	Calculated
Log Pow	2.87
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Syracuse Research Corporation (SRC)

Substance Name	cis-2-Pinanol
CAS No.	4948-28-l
Method/guideline	Calculated
Log Pow	2.98
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Syracuse Research Corporation (SRC)

Substance Name	2-Pinanol
CAS No.	473-54-l
Method/guideline	Calculated
Log **Pow**	2.98
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Syracuse Research Corporation (SRC)

Substance Name	*trans*-2-Pinanol
CAS No.	4948-29-2
Method/guideline	Calculated
Log Pow	2.85

Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions,
References	Syracuse Research Corporation (SRC)

Substance Name	2-Pinanol hydroperoxide
CAS No.	28324-52-9
Method/guideline	Calculated based on degradation to 2-pinanol
Log Pow	**2.85**
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
General Remarks	Based on degradation to 2-Pinanol
References	Syracuse Research Corporation (SRC)

Substance Name	Pine oil
CAS No.	**8002-09-3**
Method/guideline	Calculated based on principal constituents
Log Pow	**2.9**
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
General Remarks	Calculation based on principle components
References	Syracuse Research Corporation (SRC)

Substance Name	Linalool
CAS No.	**78-70-6**
Method/guideline	Measured (Karickhoff and Brown method, 1979)
GLP	**NG**
Year	1995
Log Pow	**2.97**
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Misra G., Pavlostathis S.G., Li J., and Perdue E. M. (1995) Characterization and Biodegradation of Selected Monoterpenes. 68th Annual Conference & Exposition, Water Environment Federation; Miami Beach, FL.

Substance Name	alpha-Terpineol
CAS No.	98-55-5
Method/guideline	Measured (Karickhoff and Brown method, 1979)
GLP	**NG**
Year	**1995**
Log Pow	2.98
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Misra G., Pavlostathis S.G., Li J., and Perdue E. M. (1995) Characterization and Biodegradation of Selected Monoterpenes. 68th Annual Conference & Exposition, Water Environment Federation; Miami Beach, FL.

Substance Name	2,6,6-Trimethylbicyclo[3.1 .1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl alcohol)
CAS No.	125252-49-5
Method/guideline	Measured (Karickhoff and Brown method, 1979)
GLP	**NG**
Year	1995
Log Pow	2.87
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Misra G., Pavlostathis S.G., Li J., and Perdue E. M. (1995) Characterization and Biodegradation of Selected Monoterpenes. 68th Annual Conference & Exposition, Water Environment Federation; Miami Beach, FL.

1.5 Water Solubility

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)
CAS No.	125252-49-5
Method/guideline	The determination was carried out using the flask method, Method A6 of Commission Directive 92/69/EEC (which constitutes Annex V of Council Directive 67/548/EEC).
GLP	**Yes**
Year	1997

Remarks for Test Conditions	An aliquot (0.2674) of test material was diluted with glass double distilled waster (100 ml). After shaking at 30 °C for approximately 25-1/2 hours and standing at 20 °C for approximately 24 1/2 hours, solution was filtered and analyzed.
Value (mg/L) at Temperature	60.5 mg/l at 20.0 +/- 0.5 °C
pH value and Concentration	6.3
Conclusion Remarks	The water solubility of Plinyl Acetate was determined to be 6.05 X 10E-2 g/l of solution at 20.0 +/- 0.5 °C.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliabilities Remarks	The study was performed in compliance with the UK GLP and these Principles are in accordance with GLP standard published as OECD Environment Monograph No. 45 (OECD/GD(92)32).
References	Lumsden A. M. (1998) Plinyl Acetate: Determination of general physico-chemical properties. Safepharm Laboratories, Inc. SPL Project Number: 1044/001.

Substance Name	Linalool
CAS No.	78-70-6
GLP	NA
Value (mg/L) at Temperature	1450 mg/l at 20 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions,
References	Givaudan Roure (1991a) Determination of ready biodegradability of linalool. Unpublished report.

Substance Name	Linalyl acetate
CAS No.	115-95-7
GLP	NA
Value (mg/L) at Temperature	30 mg/l (no temperature assigned)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Flavor and Extract Manufacturers' Association (FEMA) (1998) Report on the metabolism of linalyl acetate in rat tissue & intestinal homogenates. Unpublished report.

Substance Name	Linalyl acetate
CAS No.	115-95-7
GLP	NA
Value (mg/L) at Temperature	140 mg/L @ 20 °C

Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Givaudan Roure (1991c) Determination of the ready biodegradability of linalyl acetate synthetic. Unpublished report.

Substance Name	Tetrahydrolinalool
CAS No.	**78-69-3**
GLP	NA
Value (mg/L) at Temperature	700 mg/l (no temperature assigned)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Bush Boake Allen (BBA) (1990). Unpublished report to RIFM.

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
GLP	NA
Value (mg/L) at Temperature	29,000 mg/l water at 100 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Merck Index (1997) Merck & Co., inc. Publishers: Merck Research Laboratories, 12th edition, Whitehouse Station, NJ.

Substance Name	Pine oil (62.7% alpha-terpineol, 83.4% total terpene alcohol content)
CAS No.	**8002-09-3**
GLP	NA
Value (mg/L) at Temperature	Insoluble in water
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Graves, W. C. and Swigert, J. P (1994a). Pine Oil: 96-Hours Flow-through Acute Toxicity Test with Bluegill (Lepomis macrochirus). Wildlife International Ltd Report to The CSMA Pine Oil Joint Venture. Lab Project ID/Study Number 274A-101.

Substance Name	Linalool
CAS No.	78-70-6
GLP	NA
Year	1995

Remarks for Test Conditions	Water solubility determined at two temperature ranges.
Value (mg/L) at Temperature	560 mg/l at 4-8 °C and 867 mg/l at 22-25 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions,
References	Misra G., Pavlostathis S.G., Li J., and Perdue E. M. (1995) Characterization and Biodegradation of Selected Monoterpenes. 68th Annual Conference & Exposition, Water Environment Federation; Miami Beach, FL.

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
GLP	NA
Year	**1995**
Remarks for Test Conditions	Water solubility determined at two temperature ranges.
Value (mg/L) at Temperature	341 mg/l at 4-8 °C and 716 mg/l at 22-25 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Misra G., Pavlostathis S.G., Li J., and Perdue E. M. (1995) Characterization and Biodegradation of Selected Monoterpenes. 68th Annual Conference & Exposition, Water Environment Federation; Miami Beach, FL.

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)
CAS No.	125252-49-5
GLP	NA
Year	1995
Remarks for Test Conditions	Water solubility determined at two temperature ranges.
Value (mg/L) at Temperature	818 mg/l at 4-8 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Misra G., Pavlostathis S.G., Li J., and Perdue E. M. (1995) Characterization and Biodegradation of Selected Monoterpenes. 68th Annual Conference & Exposition, Water Environment Federation; Miami Beach, FL.

Substance Name	cis-2-Pinanol
CAS No.	4948-28-l

Method/guideline	Calculated at log Kow=2.85 (ESPKOW)
Value (mg/L) at temperature	**863** mg/L at 25 °C
Remarks for Data Reliability	Comparable to guidelines/standards
References	ESPOW

Substance Name	alpha-Terpineol
CAS No.	98-55-5
Method/guideline	Calculated at log Kow=2.98 (ESPKOW)
Value (mg/L) at temperature	**670** mg/L at 25 °C
Remarks for Data Reliability	Comparable to guidelines/standards
References	ESPOW

Substance Name	alpha-Terpineol acetate
CAS No.	**98-55-5**
Method/guideline	Calculated at log Kow=4.34 (ESPKOW)
Value (mg/L) at temperature	**9.03** mg/L at 25 °C
Remarks for Data Reliability	Comparable to guidelines/standards
References	ESPOW

Substance Name	Dihydromyrcenol
CAS No.	**18479-58-8**
Method/guideline	Calculated at log Kow=3.47 (ESPKOW)
Value (mg/L) at temperature	**252** mg/L at 25 °C
Remarks for Data Reliability	Comparable to guidelines/standards
References	ESPOW

Substance Name	Linalool
CAS No.	**78-70-6**
Method/guideline	Calculated at log Kow=2.97 (ESPKOW)

Value (mg/L) at temperature	684 mg/L at 25 °C
Remarks for Data Reliability	Comparable to guidelines/standards
References	ESPOW

Substance Name	Linalyl acetate
CAS No.	**115-95-7**
Method/guideline	Calculated at log Kow=4.39 (ESPKOW)
Value (mg/L) at temperature	8.20 mg/L at 25 °C
Remarks for Data Reliability	Comparable to guidelines/standards
References	ESPOW

Substance Name	Myrcenol
CAS No.	**543-39-5**
Method/guideline	Calculated at log Kow=3.46 (ESPKOW)
Value (mg/L) at temperature	261 mg/L at 25 °C
Remarks for Data Reliability	Comparable to guidelines/standards
References	ESPOW

Substance Name	Pinane hydroperoxide
CAS No.	**28324-52-9**
Method/guideline	Calculated at log Kow=3.02 (ESPKOW)
Value (mg/L) at temperature	160 mg/L at 25 °C
Remarks for Data Reliability	Comparable to guidelines/standards
References	ESPOW

Substance Name	Tetrahydrolinalool
CAS No.	**78-69-3**
Method/guideline	Calculated at log Kow=3.60 (ESPKOW)
Value (mg/L) at temperature	189 mg/L at 25 °C

Remarks for Data Reliability	Comparable to guidelines/standards
References	ESPOW

2 Environmental Fate and Pathways

2.1 Photodegradation

Substance Name	cis-2-Pinanol
CAS No.	4948-28-l
Method/guideline	Calculation
Test Type	AOPWIN
Halflife t1/2	9.08 hrs
Data Reliabilities Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
References	AOPWIN

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Method/guideline	Calculation
Test **Type**	AOPWIN
Halflife t1/2	1.24 hrs
Data Reliabilities Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
References	AOPWIN

Substance Name	alpha-Terpineol acetate
CAS No.	80-26-2
Method/guideline	Calculation
Test Type	AOPWIN
Halflife t1/2	1.35 hrs
Data Reliabilities Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
References	AOPWIN

Substance Name	Dihydromyrcenol
CAS No.	18479-58-8
Method/guideline	Calculation
Test Type	AOPWIN
Halflife t1/2	3.45 hrs
Data Reliabilities Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
References	AOPWIN

Substance Name	Linalool
CAS No.	78-70-6
Method/guideline	Calculation
Test Type	AOPWIN
Halflife t1/2	1.07 hrs
Data Reliabilities Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
References	AOPWIN

Substance Name	Linalyl acetate
CAS No.	115-95-7
Method/guideline	Calculation
Test Type	AOPWIN
Halflife t1/2	1.10 hrs
Data Reliabilities Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
References	AOPWIN

Substance Name	Myrcenol
CAS No.	543-39-5
Method/guideline	Calculation

Test Type	AOPWIN
Halflife t1/2	1.14 hrs
Data Reliabilities Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
References	AOPWIN

Substance Name	Pinane hydroperoxide
CAS No.	28324-52-9
Method/guideline	Calculation
Test Type	AOPWIN
Halflife t1/2	6.80 hrs (NOTE: these data are for 2-Pinanol)
Data Reliabilities Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
References	AOPWIN

Substance Name	Tetrahydrolinalool
CAS No.	**78-69-3**
Method/guideline	Calculation
Test Type	AOPWIN
Halflife t1/2	8.99 hrs
Data Reliabilities Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
References	AOPWIN

2.2 Stability in Water

Substance Name	Linalyl acetate
CAS No.	**115-95-7**
Method/guideline	Hydrolysis in artificial gastric juice
GLP	**No**

Year	1999
Duration (days)	3 hrs
Analytical procedures	At 37 C, 50 ml of artificial gastric juice adjusted to pH 1.2 or 7.0 was incubated with 50uM linalyl acetate in DMSO with DMSO 0.2%(v/v) of the final mixture. Experiments in acidic gastric juice were performed with and without peptic enzymes. Sample were withdrawn at intervals beginning at 0.1 minutes and ending at 180 minutes and analyzed by Chromopack CP-9003 gas chromatograph.
Temperature	37 °C
Rate constant	Rate constant k=0.006 min-1 at pH=7.0; rate constant k=>3.5 min-1 at pH=1.2 without enzyme; rate constant k=>3.5 min-1 at pH=1.2 with enzyme.
Halflife t1/2	t(1/2)=112.3 min. at pH=7.0: t(1/2)=<2.5 min. at pH=1.2 ,no enzyme; t(1/2)=<2.5 min. at pH=1.2 ,with enzyme
Breakdown products	Linalool and acetic acid formed under all conditions. At different pH with or without enzyme, linalool reacted to form alpha-terpineol in approximately equal amount. Small amounts of geraniol also formed.
Conclusion remarks	Linalyl acetate readily hydrolyzes in neutral and acidic media. The hydrolysis product linalool subsequent partially rearranges to alpha-terpineol and to a lesser extent, geraniol.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	Experiments performed with all necessary internal and external standards. Study evaluated the hydrolysis of at least 20 substrates.
References	Buck N. R. and Renwick A.G. (1999) Hydrolysis of tertiary terpenoid esters in artificial gastric juice and intestinal fluid. University of Southampton. Private Communication to FEMA. Unpublished Report.

Substance Name	Linalyl acetate
CAS No.	115-95-7
Method/guideline	Hydrolysis in artificial intestinal fluid
GLP	No
Year	1999
Duration (days)	3 hrs
Analytical procedures	At 37 C, 50 ml of artificial intestinal fluid adjusted to pH 7.5 was incubated with 50uM linalyl acetate in DMSO with DMSO 0.2%(v/v) of the final mixture. Experiments in intestinal fluid were performed with and without pancreatin enzymes. Sample were withdrawn at intervals beginning at 0.1 minutes and ending at 180 minutes and analyzed by Chromopack CP gas chromatography.
Temperature	37 °C

Rate constant	Rate constant k=0.007 min-1 at pH=7.5 without enzyme; rate constant k=0.008 min-1 at pH=7.5 with enzyme;
Halflife t1/2	t(1/2)=96.8 min. at pH=7.5 ,no pancreatin enzyme; t(1/2)=83.1 min. at pH=7.5 ,with enzyme.
Breakdown products	Linalool and acetic acid formed under all conditions. At different pH with or without enzyme, linalool reacted to form alpha-terpineol and smaller amounts of geraniol and nerol.
Conclusion remarks	Linalyl acetate readily hydrolyzes in neutral media. The hydrolysis product linalool subsequent partially rearranges to alpha-terpineol and to a lesser extent, geraniol and geraniol.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	Experiments performed with all necessary internal and external standards. Study evaluated the hydrolysis of at least 20 substrates.
References	Buck N. R. and Renwick A.G. (1999) Hydrolysis of tertiary terpenoid esters in artificial gastric juice and intestinal fluid. University of Southampton. Private Communication to FEMA. Unpublished Report.

Substance Name	*alpha* Terpineol acetate
CAS No.	80-26-2
Method/guideline	Hydrolysis in artificial gastric juice
GLP	No
Year	1999
Duration (days)	3hrs
Analytical procedures	At 37 C, 50 ml of artificial gastric juice adjusted to pH 1.2 or 7.0 was incubated with 50uM alpha-terpineol acetate in DMSO with DMSO 0.2%(v/v) of the final mixture. Experiments in acidic gastric juice were performed with and without peptic enzymes. Sample were withdrawn at intervals beginning at 0.1 minutes and ending at 180 minutes and analyzed by Chromopack CP-9003 gas chromatograph.
Temperature	37 °C
Rate constant	Rate constant k=0.00081 min-1 at pH=7.0; rate constant k=0.038 min-1 at pH=1.2 without enzyme; rate constant k=0.042 min-1 at pH=1.2 with enzyme.
Halflife t1/2	t(1/2)=859.7 min. at pH=7.0: t(1/2)=18.3 min. at pH=1.2 ,no enzyme; t(1/2)=16.4 min. at pH=1.2 ,with enzyme
Breakdown products	alpha-Terpineol acetate is hydrolyzed to alpha-terpineol and acetic acid.
Conclusion remarks	alpha-Terpineol readily hydrolyzes to alpha-terpineol and acetic acid in acidic and neutral media.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	Experiments performed with all necessary internal and external standards. Study evaluated the hydrolysis of at least 20 substrates.

References	Buck N. R. and Renwick A.G. (1999) Hydrolysis of tertiary terpenoid esters in artificial gastric juice and intestinal fluid. University of Southampton. Private Communication to FEMA. Unpublished Report.

Substance Name	alpha Terpineol acetate
CAS No.	80-26-2
Method/guideline	Hydrolysis in artificial intestinal fluid
GLP	No
Year	1999
Duration (days)	3hrs
Analytical procedures	At 37 C, 50 ml of artificial intestinal fluid adjusted to pH 7.5 was incubated with 50uM alpha-terpineol acetate in DMSO with DMSO 0.2%(v/v) of the final mixture. Experiments in intestinal fluid were performed with and without pancreatin enzymes. Sample were withdrawn at intervals beginning at 0.1 minutes and ending at 180 minutes and analyzed by Chromopack CP gas chromatograph.
Temperature	37 °C
Rate constant	Rate constant k=0.002 min-1 at pH=7.5 without enzyme; rate constant k=0.002 min-1 at pH=7.5 with enzyme;
Halflife t1/2	t(1/2)=358.2 min. at pH=7.5 ,no pancreatin enzyme; t(1/2)=371.5 min. at pH=7.5 ,with enzyme.
Breakdown products	alpha-Terpineol acetate is hydrolyzed to alpha-terpineol and acetic acid.
Conclusion remarks	alpha-Terpineol readily hydrolyzes to alpha-terpineol and acetic acid in neutral media.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	Experiments performed with all necessary internal and external standards. Study evaluated the hydrolysis of at least 20 substrates.
References	Buck N. R. and Renwick A.G. (1999) Hydrolysis of tertiary terpenoid esters in artificial gastric juice and intestinal fluid. University of Southampton. Private Communication to FEMA. Unpublished Report.

2.3 Biodegradation

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)
CAS No.	125252-49-5
Method/guideline	The method followed that described in the OECD Guidelines for testing of Chemicals (1992) No. 301 F, "Readv Biodeoradabilitv;

	testing of Chemicals (1992) No. 301F, "Ready Biodegradability; Monometric Respiratory Test" referenced as Method C.4D of Commission Directive 92/69/EEC.
Test Type	Monometric Respiratory Test
GLP	**Yes**
Year	1997
Contact Time	**28** days
Innoculum	Activated sludge
Remarks for Test Conditions	100 mg DOC/l at 21 C for 28 days
Degradation % After Time	**6%** at 28 days
Results	**6%** after 28 days
10 day Window Criteria	**No**
Total degradation	**No**
Conclusion Remarks	Cannot be considered to be readily biodegradable under the terms and conditions of OECD guideline No. 301 F.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	The Study was performed in compliance with UK GLP standards. These regulations are in accordance with GLP standard published as OECD monograph No. 45.
Reference	Mead C. (1997b) Plinyl acetate: Assessment of Ready Biodegradability; Manometric Respiratory Test. Safepharm Laboratories, Ltd. SPL Project No. 1044/015.

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)
CAS No.	**125252-49-5**
Method/guideline	The method followed that described in the OECD Guidelines for Testing of Chemicals (1984) No. 209 "Activated Sludge Respiration Inhibition Test" and EEC Commission Directive 87/302/EEC.
Test **Type**	Activated Sludge Respiration inhibition Test.
GLP	**Yes**
Year	**1997**
Contact Time	3 hours
Innoculum	Activated Sludge from sewage treatment plant in UK
Remarks for Test Conditions	The test material was aerated for a period of 3 hours at 21 C in the presence of activated sewage sludge with the addition of a synthetic sewage a respiratory substrate. The rate of respiration was determined after 30 min and 3 hours contact time.

Results	The effect of the test material on the respiration of activated sludge gave a 3-hour EC50 of 360 mg/l. The NOEC was determined to be 100 mg/l
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	The study was performed in compliance with UK GLP standard. These regulations are in accordance with GLP Standards published as OECD Monograph No. 45 (OCDE/GD(92)32).
Reference	Mead C. (1997c) Plinyl acetate: Assessment of the Inhibitory Effect on the Respiration of Activated Sewage Sludge. Safepharm Laboratories. SPL Project No. 1044/018.

Substance Name	Linalool Synthetic, 97.6% pure (GLC)
CAS No.	78-70-6
Method/guideline	Ready biodegradability was determined by modified MITI test, OECD guideline
Test Type	Modified MITI test
GLP	NG
Year	1991
Contact Time	28 days
Innoculum	Activated sludge from city waste water treatment plant
Remarks for Test Conditions	Activated sludge was prepared by mixing sludge from biological waste water treatment plant & soil sampled on the bank of the river. Reference Substance: Aniline. Activated sludge conc. 30 mg/l, test substance 100 mg/l, reference substance 100 mg/l.
Degradation % After Time	80% at 28 days for test chemical, for aniline: 79%
Results	80% biodegradation in 28 days.
Total degradation	No
Conclusion Remarks	Linalool synthetic is readily biodegradable under the test conditions.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	The study followed OECD guidelines.
Reference	Rudio J. (1991) Test Report Nr 90-57/B. Linalool Synthetic. Biodegradation unpublished report.

Substance Name	Linalool
CAS No.	78-70-6
Method/guideline	The sealed vessel test is a CO_2 production test based on OECD Guideline 301 B(1)
Test Type	Sealed Vessel Test

GLP	**Yes**
Year	**1990**
Contact Time	28 days
Innoculum	Secondary effluent from an unacclimatized activated sludge plant at URL North
Remarks for Test Conditions	Test is conducted in a 160 ml vessel containing 100 ml mineral salt medium inoculated with secondary effluent and the respective test or reference material. The sealed vessels are incubated at 20 C on a rotary shaker for 28 days.
Degradation % After Time	97.1%
Results	97.1% (95% confidence interval 85.0 - 109.3)
Time required for 10% Degradation	< 4 days
10 day Window Criteria	Yes
Conclusion Remarks	The test material was readily and ultimately biodegradable.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	The study was conducted in accordance with GLP and OECD guideline.
Reference	Quest International Ltd. (1994d) Biodegradability test of linalool in a sealed vessel test. Unpublished report.

Substance Name	Pine oil (disinfectant) (mixture contains 50-60% alpha-terpineol and 10-l 5% other terpineol isomers)
CAS No.	**8002-09-3**
Method/guideline	Biodegradability and biochemical oxygen demand.
Test Type	Biodegradability
GLP	NG
Year	1966
Contact Time	20 days
Innoculum	Activated sludge
Degradation % After Time	Not given
Results	Biological Oxygen demand (5 days)= 0.8 mglml; COD=1.60 mglml; chemical oxygen demand of organic feed to activated sludge = 428 mglml; BOD 5-day of feed to activated sludge units= 255 mglml; loading on activated sludge units= 47.8.
Data Qualities Reliabilities	Biodegradability cannot be determined from the limited data in this report.
Reference	Ryckman, Edgerley, Burbank and Associates, Inc. (1966) Unpublished report to Hercules Powder Company.

Substance Name	Myrcenol
CAS No.	543-39-5
Method/guideline	OECD closed bottle shake flask activated sludge biodegradation in soil.
Test Type	20 day biochemical oxygen demand
GLP	NG(62.7% alpha-terpineol, 83.4% total terpene alcohol content)
Year	1986
Innoculum	Activated sludge
Remarks for Test Conditions	Myrcenol was added by syringe, injected directly into BOD bottle due to limited solubility.
Degradation % After Time	**66%** in 20 days
Time required for 10% Degradation	<10 days
10 day Window Criteria	Yes
Conclusion Remarks	Myrcenol is biodegradable.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	The study was conducted in accordance with OECD guideline.
Reference	UCC Business Confidential (1986) Ecological Fate and Effects Testing of UCC Products and Wastewaters During 1985.

Substance Name	alpha-Terpineol acetate (100%)
CAS No.	**80-26-2**
Method/guideline	The method followed that described in the OECD Guidelines for testing of Chemicals (1992) No. 301F, "Ready Biodegradability; Monometric Respiratory Test" referenced as Method C.4-D of Commission Directive 92/69/EEC.
Test Type	Monometric Respiratory Test
GLP	**Yes**
Year	**1996**
Contact Time	**28** days
Innoculum	Activated sludge
Remarks for Test Conditions	30 mg/L activated sludge, 100 mg/L test substance or reference (aniline) material were incubated for 28 days at 20 °C.
Degradation % After Time	**63%** after 28 days
Results	63% of the test substance was biodegraded in 28 day whereas 79% of reference material (aniline) was biodegraded during the same period.

10 day Window Criteria	**No**
Conclusion Remarks	alpha-Terpinyl acetate was biodegradable under the test conditions.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	The study was conducted in accordance with OECD guideline.
Reference	Givaudan Roure (1996b) Ready biodegradability of *alpha*-terpineol acetate. Unpublished report.

Substance Name	alpha-Terpineol acetate
CAS No.	80-26-2
Method/guideline	The sealed vessel test is a CO_2 production test based on OECD Guideline 301 B(1)
Test Type	Sealed Vessel Test
GLP	Yes
Year	1994
Contact Time	28 days
Innoculum	Secondary effluent from an unacclimatized activated sludge plant at URL North
Remarks for Test Conditions	Test is conducted in a 160 ml vessel containing 100 ml mineral salt medium inoculated with secondary effluent and the respective test or reference material. The sealed vessels are incubated at 20 °C on a rotary shaker for 28 days.
Degradation % After Time	87.3% after 28 days
Results	87.3% (95% confidence interval 85.889%)
10 day Window Criteria	Yes
Conclusion Remarks	The test material was readily and ultimately biodegradable.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	The study was conducted in accordance with GLP and OECD guideline.
Reference	Quest International Ltd. (1994a) Biodegradability test of terpinyl acetate in a sealed vessel test. Private communication to RIFM.

Substance Name	Tetrahydrolinalool (98%)
CAS No.	**78-69-3**
Method/guideline	The sealed vessel test is a CO_2 production test based on OECD Guideline 301 B(1).
Test **Type**	Sealed Vessel Test
GLP	**Yes**

Year	1994
Contact Time	28 days
Innoculum	Secondary effluent from an unacclimatized activated sludge plant at URL North
Remarks for Test Conditions	Test is conducted in a 160 ml vessel containing 100 ml mineral salt medium inoculated with secondary effluent and the respective test or reference material. The sealed vessels are incubated at 17-22 °C on a rotary shaker for 28 days.
Degradation % After Time	103.1 %after 28 days
Results	103.1% (95% confidence interval 986107.7%)
10 day Window Criteria	Yes
Conclusion Remarks	The test material was readily and ultimately biodegradable.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	The study was conducted in accordance with GLP and OECD guideline.
Reference	Quest International Ltd. (1994b) The ultimate biodegradability of tetrahydrolinalool in the sealed vessel test. Private communication to RIFM.

Substance Name	Linalyl acetate (96.0%)
CAS No.	**115-95-7**
Method/guideline	Ready Biodegradability was determined by modified MITI test, OECD guideline.
Test **Type**	Modified MITI test
GLP	**Yes**
Year	1991
Contact Time	28 days
Innoculum	Activated sludge from city waste water treatment plant.
Remarks for Test Conditions	Activated sludge was prepared by mixing sludge from biological waste water treatment plant & soil sampled on the bank of the river. Reference Substance: Aniline. Activated sludge conc. 30 mg/l, test substance 100 mg/l, ref. substance (aniline) 100 mg/l.
Degradation % After Time	75% after 28 days
Results	75% biodegradation in 28 days.
Conclusion Remarks	The test material was biodegradable.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	The study followed OECD guidelines.

Reference	Quest International Ltd. (1991) Biodegradability study of linalyl acetate in a sealed vessel test. Private communication to RIFM.

Substance Name	Dihydromyrcenol
CAS No.	18479-58-8
Method/guideline	The sealed vessel test is a CO2 production test based on OECD Guideline 301 B(1).
Test Type	Sealed Vessel Test
GLP	Yes
Year	1991
Contact Time	28 days
Innoculum	Secondary effluent from an unacclimatized activated sludge plant at URL North.
Remarks for Test Conditions	Test is conducted in a 160 ml vessel containing 100 ml mineral salt medium inoculated with secondary effluent and the respective test or reference material. The sealed vessels are incubated at 20 C on a rotary shaker for 28 days.
Degradation % After Time	72.1% after 28 days
Results	72.1% (95% confidence interval 68.8-75.4%)
Conclusion Remarks	The test material was biodegradable.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	The study was conducted in accordance with GLP and OECD guideline.
Reference	Quest International Ltd. (1994c) Biodegradability study of dimyrcetol in a sealed vessel test. Private comm. to RIFM.

2.4 Fugacity

Substance Name	Linalool
CAS No.	78-70-6
Model Conditions	25 °C, 100,000 lbs
Test **Type**	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP

Media	Air-Water Partition Coefficient
Absorption coefficient	**0.0029**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalool
CAS No.	**78-70-6**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP
Media	Soil-Water Partition Coefficient
Absorption coefficient	15.6
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalool
CAS No.	78-70-6
Model Conditions	25 "C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay

Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP
Media	Sediment-Water Partition Coefficient
Absorption coefficient	31.3
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalool
CAS No.	78-70-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2. 11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP
Media	Suspended Sediment-Water Partition Coefficient
Absorption coefficient	97.7
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalool
CAS No.	78-70-6
Model Conditions	25 °C, 100,000 lbs

Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP
Media	Fish-Water Partition Coefficient
Estimated Distribution and Media Concentration	**39.7**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalool
CAS No.	**78-70-6**
Model Conditions	**25** °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP
Media	Aerosol-Air Partition Coefficient
Absorption coefficient	**89600**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalool

CAS No.	**78-70-6**
Model Conditions	**25 °C,** 100,000 **lbs**
Test **Type**	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP
Media	Air
Estimated Distribution and Media Concentration	**0.455**
Data Qualities Reliabilities	Reliable with restriction
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalool
CAS No.	78-70-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP
Media	Water
Estimated Distribution and Media Concentration	0.317
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalool
CAS No.	78-70-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP
Media	Soil
Estimated Distribution and Media Concentration	0.223
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2. 11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalool
CAS No.	78-70-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP
Media	Sediment
Estimated Distribution and Media Concentration	**0.005**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.

References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalool
CAS No.	78-70-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP
Media	Suspended Sediment
Estimated Distribution and Media Concentration	**0.00015**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalool
CAS No.	78-70-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP
Media	Fish
Estimated Distribution and Media Concentration	0.000013
Data Qualities Reliabilities	Reliable with restriction.

Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalool
CAS No.	78-70-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP
Media	Aerosol
Estimated Distribution and Media Concentration	0.00000082
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Myrcenol
CAS No.	543-39-5
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Air-Water Partition Coefficient

Absorption coefficient	0.0016
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Myrcenol
CAS No.	**543-39-5**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Soil-Water Partition Coefficient
Absorption coefficient	56.7
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Myrcenol
CAS No.	**543-39-5**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I

Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Sediment-Water Partition Coefficient
Absorption coefficient	113.5
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Myrcenol
CAS No.	**543-39-5**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Suspended Sediment-Water Partition Coefficient
Absorption coefficient	**354.7**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Myrcenol
CAS No.	**543-39-5**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model

Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Fish-Water Partition Coefficient
Absorption coefficient	144.2
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Myrcenol
CAS No.	**543-39-5**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Aerosol-Air Partition Coefficient
Absorption coefficient	**895000**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Myrcenol
CAS No.	**543-39-5**

Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Air
Estimated Distribution and Media Concentration	0.181
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Myrcenol
CAS No.	**543-39-5**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Water
Estimated Distribution and Media Concentration	0.227
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Myrcenol
CAS No.	**543-39-5**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Soil
Estimated Distribution and Media Concentration	**0.579**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Myrcenol
CAS No.	**543-39-5**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP
Media	Sediment
Estimated Distribution and Media Concentration	**0.0129**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D.

(1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Myrcenol
CAS No.	**543-39-5**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Suspended Sediment
Estimated Distribution and Media Concentration	**0.00042**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Myrcenol
CAS No.	**543-39-5**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Fish
Estimated Distribution and Media Concentration	**0.000033**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or

	metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Myrcenol
CAS No.	**543-39-5**
Model Conditions	**25** °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Aerosol
Estimated Distribution and Media Concentration	**0.0000032**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Dihydromyrcenol
CAS No.	**18479-58-8**
Model Conditions	**25** °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, VP, water solubility, MP
Media	
Absorption coefficient	

Estimated Distribution and Media Concentration	
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Dihydromyrcenol
CAS No.	**18479-58-8**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, VP, water solubility, MP
Media	Air-Water Partition Coefficient
Absorption coefficient	0.0017
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Dihydromyrcenol
CAS No.	18479-58-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I

Input Parameters	MW, estimated log Kow, VP, water solubility, MP
Media	Soil-Water Partition Coefficient
Absorption coefficient	58.1
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Dihydromyrcenol
CAS No.	18479-58-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
input Parameters	MW, estimated log Kow, VP, water solubility, MP
Media	Sediment-Water Partition Coefficient
Absorption coefficient	116
Data Qualities Reliabilities	Reliable with restriction
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Dihydromyrcenol
CAS No.	**18479-58-8**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model

Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, VP, water solubility, MP
Media	Suspended Sediment-Water Partition Coefficient
Absorption coefficient	363
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Dihydromyrcenol
CAS No.	**18479-58-8**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, VP, water solubility, MP
Media	Fish-Water Partition Coefficient
Absorption coefficient	148
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Dihydromyrcenol
CAS No.	**18479-58-8**

Model Conditions	25 ❑ 'C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, VP, water solubility, MP
Media	Aerosol-Air Partition Coefficient
Absorption coefficient	895000
Data Qualities Reliabilities	Reliable with restriction,
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Dihydromyrcenol
CAS No.	**18479-58-8**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, VP, water solubility, MP
Media	Air
Estimated Distribution and Media Concentration	0.186
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Dihydromyrcenol
CAS No.	18479-58-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, VP, water solubility, MP
Media	Water
Estimated Distribution and Media Concentration	**0.222**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Dihydromyrcenol
CAS No.	**18479-58-8**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, VP, water solubility, MP
Media	Soil
Estimated Distribution and Media Concentration	**0.579**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, **D.**

	(1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Dihydromyrcenol
CAS No.	**18479-58-8**
Model Conditions	**25** "C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, VP, water solubility, MP
Media	Sediment
Estimated Distribution and Media Concentration	**0.0129**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Dihydromyrcenol
CAS No.	**18479-58-8**
Model Conditions	**2.5** °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, VP, water solubility, MP
Media	Suspended Sediment
Estimated Distribution and Media Concentration	**0.0004**
Data Qualities Reliabilities	Reliable with restriction
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or

	metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Dihydromyrcenol
CAS No.	**18479-58-8**
Model Conditions	**25** °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, VP, water solubility, MP
Media	Fish
Estimated Distribution and Media Concentration	**0.000033**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Dihydromyrcenol
CAS No.	**18479-58-8**
Model Conditions	**25** °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, VP, water solubility, MP
Media	Aerosol
Estimated Distribution and Media Concentration	**0.0000033**

Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalyl Acetate
CAS No.	115-95-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, water solubility, estimated log Kow, MP
Media	Air-Water Partition Coefficient
Absorption coefficient	**0.0062**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalyl Acetate
CAS No.	115-95-7
Model Conditions	**25** °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, water solubility, estimated log Kow, MP

Media	Soil-Water Partition Coefficient
Absorption coefficient	**483**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalyl Acetate
CAS No.	**115-95-7**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, water solubility, estimated log Kow, MP
Media	Sediment-Water Partition Coefficient
Absorption coefficient	**966**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalyl Acetate
CAS No.	115-95-7
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay

Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, water solubility, estimated log Kow, MP
Media	Suspended Sediment-Water Partition Coefficient
Absorption coefficient	**3020**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalyi Acetate
CAS No.	**115-95-7**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	**EQC** V 2.11 Level I
Input Parameters	MW, VP, water solubility, estimated log Kow, MP
Media	Fish-Water Partition Coefficient
Absorption coefficient	1230
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.1 1. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalyl Acetate
CAS No.	115-95-7
Model Conditions	25 °C, 100,000 lbs

Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, water solubility, estimated log Kow, MP
Media	Aerosol-Air Partition Coefficient
Absorption coefficient	545000
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalyl Acetate
CAS No.	**115-95-7**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, water solubility, estimated log Kow, MP
Media	Air
Estimated Distribution and Media Concentration	0.118
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalyl Acetate

CAS No.	**115-95-7**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, water solubility, estimated log Kow, MP
Media	Water
Estimated Distribution and Media Concentration	0.038
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalyl Acetate
CAS No.	115-95-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, water solubility, estimated log Kow, MP
Media	Soil
Estimated Distribution and Media Concentration	0.825
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalyl Acetate
CAS No.	115-95-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, water solubility, estimated log Kow, MP
Media	Sediment
Estimated Distribution and Media Concentration	0.0183
Data Qualities Reliabilities	Reliable with restriction
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalyl Acetate
CAS No.	115-95-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, water solubility, estimated log Kow, MP
Media	Suspended Sediment
Estimated Distribution and Media Concentration	0.00057
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.

References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalyl Acetate
CAS No.	**115-95-7**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, water solubility, estimated log Kow, MP
Media	Fish
Estimated Distribution and Media Concentration	**0.000047**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by **a** recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Linalyl Acetate
CAS No.	115-95-7
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, water solubility, estimated log Kow, MP
Media	Aerosol
Estimated Distribution and Media Concentration	0.0000013
Data Qualities Reliabilities	Reliable with restriction.

Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Tetrahydrolinalool
CAS No.	**78-69-3**
Model Conditions	**25** °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, water solubility, estimated log Kow, VP, MP
Media	Air-Water Partition Coefficient
Absorption coefficient	**0.00048**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Tetrahydrolinalool
CAS No.	**78-69-3**
Model Conditions	**25** °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, water solubility, estimated log Kow, VP, MP
Media	Soil-Water Partition Coefficient

Absorption coefficient	**78.3**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Tetrahydrolinalool
CAS No.	**78-69-3**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, water solubility, estimated log Kow, VP, MP
Media	Sediment-Water Partition Coefficient
Absorption coefficient	157
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Tetrahydrolinalool
CAS No.	**78-69-3**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I

Input Parameters	MW, water solubility, estimated log Kow, VP, MP
Media	Suspended Sediment-Water Partition Coefficient
Absorption coefficient	**490**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Tetrahydrolinalool
CAS No.	**78-69-3**
Model Conditions	25 "C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	**EQC** V 2.11 Level I
Input Parameters	MW, water solubility, estimated log Kow, VP, MP
Media	Fish-Water Partition Coefficient
Absorption coefficient	199
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Tetrahydrolinalool
CAS No.	**78-69-3**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model

Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, water solubility, estimated log Kow, VP, MP
Media	Aerosol-Air Partition Coefficient
Absorption coefficient	1130000
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Tetrahydrolinalool
CAS No.	**78-69-3**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, water solubility, estimated log Kow, VP, MP
Media	Air
Estimated Distribution and Media Concentration	**0.0499**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Tetrahydrolinalool
CAS No.	78-69-3

Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
input Parameters	MW, water solubility, estimated log Kow, VP, MP
Media	Water
Estimated Distribution and Media Concentration	**0.206**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Tetrahydrolinalool
CAS No.	**78-69-3**
Model Conditions	25 °C, 100,000 lbs
Test **Type**	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, water solubility, estimated log Kow, VP, MP
Media	Soil
Estimated Distribution and Media Concentration	**0.727**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Tetrahydrolinalool
CAS No.	**78-69-3**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, water solubility, estimated log Kow, VP, MP
Media	Sediment
Estimated Distribution and Media Concentration	0.0162
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Tetrahydrolinalool
CAS No.	**78-69-3**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, water solubility, estimated log Kow, VP, MP
Media	Suspended Sediment
Estimated Distribution and Media Concentration	**0.00051**
Data Qualities Reliabilities	Reliable with restriction
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D.

	(1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Tetrahydrolinalool
CAS No.	**78-69-3**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, water solubility, estimated log Kow, VP, MP
Media	Fish
Estimated Distribution and Media Concentration	0.000041
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Tetrahydrolinalool
CAS No.	**78-69-3**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, water solubility, estimated log Kow, VP, MP
Media	Aerosol
Estimated Distribution and Media Concentration	**0.0000011**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or

	metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibriurn Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, water solubility, log Kow, VP, MP
Media	Air-Water Partition Coefficient
Absorption coefficient	**0.00046**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, water solubility, log Kow, VP, MP
Media	Soil-Water Partition Coefficient
Absorption coefficient	18.8

Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpineol
CAS No.	98-55-5
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
input Parameters	MW, water solubility, log Kow, VP, MP
Media	Sediment-Water Partition Coefficient
Absorption coefficient	37.6
Data Qualities Reliabilities	Reliable with restriction,
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, water solubility, log Kow, VP, MP

Media	Suspended Sediment-Water Partition Coefficient
Absorption coefficient	117
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, water solubility, log Kow, VP, MP
Media	Fish-Water Partition Coefficient
Absorption coefficient	47.8
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay

Model Used	EQC V 2.11 Level I
Input Parameters	MW, water solubility, log Kow, VP, MP
Media	Aerosol-Air Partition Coefficient
Absorption coefficient	1130000
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, water solubility, log Kow, VP, MP
Media	Air
Estimated Distribution and Media Concentration	0.11
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Model Conditions	25 °C, 100,000 lbs

Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, water solubility, log Kow, VP, MP
Media	Water
Estimated Distribution and Media Concentration	**0.477**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Model Conditions	**25** °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, water solubility, log Kow, VP, MP
Media	Soil
Estimated Distribution and Media Concentration	**0.404**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpineol

CAS No.	**98-55-5**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, water solubility, log Kow, VP, MP
Media	Sediment
Estimated Distribution and Media Concentration	**0.009**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, water solubility, log Kow, VP, MP
Media	Suspended Sediment
Estimated Distribution and Media Concentration	**0.00028**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, water solubility, log Kow, VP, MP
Media	Fish
Estimated Distribution and Media Concentration	**0.000023**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, water solubility, log Kow, VP, MP
Media	Aerosol
Estimated Distribution and Media Concentration	**0.0000025**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.

References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpinyl acetate
CAS No.	80-26-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, estimated water solubility, VP, MP
Media	Air-Water Partition Coefficient
Absorption coefficient	0.141
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpinyl acetate
CAS No.	80-26-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, estimated water solubility, VP, MP
Media	Soil-Water Partition Coefficient
Absorption coefficient	**393**
Data Qualities Reliabilities	Reliable with restriction.

Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpinyl acetate
CAS No.	**80-26-2**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, estimated water solubility, VP, MP
Media	Sediment-Water Partition Coefficient
Absorption coefficient	**785**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpinyl acetate
CAS No.	**80-26-2**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, estimated water solubility, VP, MP
Media	Suspended Sediment-Water Partition Coefficient

Absorption coefficient	**2450**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpinyl acetate
CAS No.	**80-26-2**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, estimated water solubility, VP, MP
Media	Fish-Water Partition Coefficient
Absorption coefficient	**998**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpinyl acetate
CAS No.	**80-26-2**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I

Input Parameters	MW, log Kow, estimated water solubility, VP, MP
Media	Aerosol-Air Partition Coefficient
Absorption coefficient	**347000**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpinyl acetate
CAS No.	80-26-2
Model Conditions	**25** °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, estimated water solubility, VP, MP
Media	Air
Estimated Distribution and Media Concentration	**0.787**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpinyl acetate
CAS No.	80-26-2
Model Conditions	**25** °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model

Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, estimated water solubility, VP, MP
Media	Water
Estimated Distribution and Media Concentration	0.0112
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpinyl acetate
CAS No.	80-26-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, estimated water solubility, VP, MP
Media	Soil
Estimated Distribution and Media Concentration	**0.197**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpinyl acetate
CAS No.	80-26-2

Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
input Parameters	MW, log Kow, estimated water solubility, VP, MP
Media	Sediment
Estimated Distribution and Media Concentration	0.0044
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpinyl acetate
CAS No.	80-26-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, estimated water solubility, VP, MP
Media	Suspended Sediment
Estimated Distribution and Media Concentration	0.00014
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpinyl acetate
CAS No.	80-26-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, estimated water solubility, VP, MP
Media	Fish
Estimated Distribution and Media Concentration	**0.000011**
Data Qualities Reliabilities	Reliable with restriction,
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.1 1. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	alpha-Terpinyl acetate
CAS No.	80-26-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, estimated water solubility, VP, MP
Media	Aerosol
Estimated Distribution and Media Concentration	0.0000055
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D.

	(1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)
CAS No.	**125252-49-5**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP
Media	Air-Water Partition Coefficient
Absorption coefficient	**0.0038**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)
CAS No.	**125252-49-5**
Model Conditions	**25 °C,** 100,000 Ibs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP
Media	Soil-Water Partition Coefficient
Absorption coefficient	**43**
Data Qualities Reliabilities	Reliable with restriction.

Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance ▪ plinyl acetate, clear colorless non-viscous liquid)
CAS No.	**125252-49-5**
Model Conditions	25 °C, 100,000 lbs
Test **Type**	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP
Media	Sediment-Water Partition Coefficient
Absorption coefficient	86.1
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance ▪ plinyl acetate, clear colorless non-viscous liquid)
CAS No.	**125252-49-5**
Model Conditions	25 °C, 100,000 lbs
Test **Type**	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP

Media	Suspended Sediment-Water Partition Coefficient
Absorption coefficient	**269**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)
CAS No.	125252-49-5
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP
Media	Fish-Water Partition Coefficient
Absorption coefficient	109
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, **D.** (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)
CAS No.	**125252-49-5**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model

Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP
Media	Aerosol-Air Partition Coefficient
Absorption coefficient	**645000**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)
CAS No.	**125252-49-5**
Model Conditions	**25** °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP
Media	Air
Estimated Distribution and Media Concentration	**0.39**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)

CAS No.	125252494
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP
Media	Water
Estimated Distribution and Media Concentration	0.205
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance ▪ plinyl acetate, clear colorless non-viscous liquid)
CAS No.	125252-49-5
Model Conditions	25 "C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP
Media	Soil
Estimated Distribution and Media Concentration	**0.397**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.1 1. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity

approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)
CAS No.	**12525249-5**
Model Conditions	**25** °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	**EQC** V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP
Media	Sediment
Estimated Distribution and Media Concentration	**0.0088**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)
CAS No.	**125252-49-5**
Model Conditions	**25** °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	**EQC** V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP
Media	Suspended Sediment
Estimated Distribution and Media Concentration	**0.00028**
Data Qualities Reliabilities	Reliable with restriction.

Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)
CAS No.	**125252-49-5**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP
Media	Fish
Estimated Distribution and Media Concentration	**0.000022**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.1 **1**. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)
CAS No.	125252-49-5
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, log Kow, water solubility, VP, MP

Media	Aerosol
Estimated Distribution and Media Concentration	**0.000005**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	*cis*-2-Pinanol
CAS No.	**4948-28-I**
Model Conditions	**25** °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Air-Water Partition Coefficient
Absorption coefficient	**0.0067**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	*cis*-2-Pinanol
CAS No.	**4948-28-I**
Model Conditions	**25** °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay

Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Soil-Water Partition Coefficient
Absorption coefficient	**13.9**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	cis-2-Pinanol
CAS No.	**4948-28-l**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Sediment-Water Partition Coefficient
Absorption coefficient	**27.9**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	*cis*-2-Pinanol
CAS No.	**4948-28-l**
Model Conditions	25 °C, 100,000 lbs

Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Suspended Sediment-Water Partition Coefficient
Absorption coefficient	87.1
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	*cis*-2-Pinanol
CAS No.	4948-28-I
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	35.4
Absorption coefficient	Fish-Water Partition Coefficient
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	*cis*-2-Pinanol

CAS No.	**4948-28-I**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Aerosol-Air Partition Coefficient
Absorption coefficient	**645000**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	cis-2-Pinanol
CAS No.	**4948-28-I**
Model Conditions	25 "C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Air
Estimated Distribution and Media Concentration	0.17
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	*cis*-2-Pinanol
CAS No.	4948-28-I
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Water
Estimated Distribution and Media Concentration	**0.506**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	cis-2-Pinanol
CAS No.	**4948-28-I**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Soil
Estimated Distribution and Media Concentration	0.317
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.

References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	*cis*-2-Pinanol
CAS No.	**4948-28-I**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Sediment
Estimated Distribution and Media Concentration	**0.007**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	cis-2-Pinanol
CAS No.	**4948-28-I**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Suspended Sediment
Estimated Distribution and Media Concentration	**0.00022**
Data Qualities Reliabilities	Reliable with restriction.

Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	*cis*-2-Pinanol
CAS No.	4948-28-l
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	**EQC** V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Fish
Estimated Distribution and Media Concentration	0.000018
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	*cis*-2-Pinanol
CAS No.	4948-28-l
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Aerosol

Estimated Distribution and Media Concentration	**0.0000022**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	*trans*-2-Pinanol
CAS No.	**4948-29-2**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Air-Water Partition Coefficient
Absorption coefficient	0.0067
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	*trans*-2-Pinanol
CAS No.	**4948-29-2**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I

Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Soil-Water Partition Coefficient
Absorption coefficient	**13.9**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	*trans*-2-Pinanol
CAS No.	**4948-29-2**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Sediment-Water Partition Coefficient
Absorption coefficient	**27.9**
Data Qualities Reliabilities	Reliable with restriction
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	*trans*-2-Pinanol
CAS No.	**4948-29-2**
Model Conditions	25 °C, 100,000 lbs
Test **Type**	Environmental Equilibrium Partitioning Model

Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Suspended Sediment-Water Partition Coefficient
Absorption coefficient	87.1
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	*trans*-2-Pinanol
CAS No.	**4948-29-2**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Fish-Water Partition Coefficient
Absorption coefficient	35.4
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	*trans*-2-Pinanol
CAS No.	**4948-29-2**

Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Aerosol-Air Partition Coefficient
Absorption coefficient	645000
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	*trans*-2-Pinanol
CAS No.	**4948-29-2**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Air
Estimated Distribution and Media Concentration	0.17
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	*trans*-2-Pinanol
CAS No.	**4948-29-2**
Model Conditions	**25 °C,** 100,000 **lbs**
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Water
Estimated Distribution and Media Concentration	**0.506**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	frans-2-Pinanol
CAS No.	**4948-29-2**
Model Conditions	**25 °C,** 100,000 lbs
Test **Type**	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Soil
Estimated Distribution and Media Concentration	**0.317**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D.

	(1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	*trans*-2-Pinanol
CAS No.	**4948-29-2**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Sediment
Estimated Distribution and Media Concentration	**0.007**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	*trans*-2-Pinanol
CAS No.	**4948-29-2**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Suspended Sediment
Estimated Distribution and Media Concentration	**0.00022**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or

	metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	*trans*-2-Pinanol
CAS No.	4948-29-2
Model Conditions	25 "C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Fish
Estimated Distribution and Media Concentration	0.000018
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.1 1. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	*trans*-2-Pinanol
CAS No.	**4948-29-2**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Aerosol
Estimated Distribution and Media Concentration	0.0000022

Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2-Pinanolhydroperoxide
CAS No.	**28324-52-9**
Model Conditions	**25 °C**, 100,000 Ibs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Air-Water Partition Coefficient
Absorption Coefficient	**0.00336**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2-Pinanolhydroperoxide
CAS No.	**28324-52-9**
Model Conditions	**25 °C**, 100,000 Ibs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP

Media	Soil-Water Partition Coefficient
Absorption Coefficient	**20.6**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2-Pinanolhydroperoxide
CAS No.	28324-52-9
Model Conditions	25 °C, 100,000 lbs
Test **Type**	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Sediment-Water Partition Coefficient
Absorption Coefficient	41.2
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2-Pinanolhydroperoxide
CAS No.	**28324-52-9**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay

Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Suspended Sediment-Water Partition Coefficient
Absorption Coefficient	**129**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2-Pinanolhydroperoxide
CAS No.	**28324-52-9**
Model Conditions	**25** °C, 100,000 Ibs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Fish-Water Partition Coefficient
Absorption Coefficient	**52.4**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2-Pinanolhydroperoxide
CAS No.	**28324-52-9**
Model Conditions	25 °C, 100,000 Ibs

Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	**EQC** V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Aerosol-Air Partition Coefficient
Absorption Coefficient	**544000**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.1 1. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2-Pinanolhydroperoxide
CAS No.	28324-52-g
Model Conditions	**25** °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Air
Estimated Distribution and Media Concentration	**0.463**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL

Substance Name	2-Pinanolhydroperoxide

CAS No.	**28324-52-9**
Model Conditions	**25 °C**, 100,000 lbs
Test **Type**	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Water
Estimated Distribution and Media Concentration	**0.276**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2-Pinanolhydroperoxide
CAS No.	**28324-52-9**
Model Conditions	**25 °C**, 100,000 lbs
Test **Type**	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Soil
Estimated Distribution and Media Concentration	**0.256**
Data Qualities Reliabilities	Reliable with restriction,
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1992) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2-Pinanolhydroperoxide 1
CAS No.	**28324-52-9**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Sediment
Estimated Distribution and Media Concentration	**0.0057**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2-Pinanolhydroperoxide
CAS No.	**28324-52-9**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Suspended Sediment
Absorption Coefficient	
Estimated Distribution and Media Concentration	0.00018
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or

	metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2-Pinanolhydroperoxide
CAS No.	**28324-52-9**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Fish
Estimated Distribution and Media Concentration	**0.000014**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	2-Pinanolhydroperoxide
CAS No.	**28324-52-9**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Aerosol
Estimated Distribution and Media Concentration	**0.000005**

Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Pine oil
CAS No.	**8002-09-3**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Air-Water Partition Coefficient
Absorption Coefficient	**0.00083**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Pine oil
CAS No.	**8002-09-3**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP

Media	Soil-Water Partition Coefficient
Absorption Coefficient	15.6
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Pine oil
CAS No.	**8002-09-3**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Sediment-Water Partition Coefficient
Absorption Coefficient	31.3
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Pine oil
CAS No.	**8002-09-3**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay

Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Suspended Sediment-Water Partition Coefficient
Absorption Coefficient	**97.7**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Pine oil
CAS No.	**8002-09-3**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Fish-Water Partition Coefficient
Absorption Coefficient	**39.7**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Pine oil
CAS No.	**8002-09-3**
Model Conditions	25 °C, 100,000 lbs

Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Aerosol-Air Partition Coefficient
Absorption Coefficient	645000
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Pine oil
CAS No.	**8002-09-3**
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Air
Estimated Distribution and Media Concentration	0.194
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.1 1. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL,

Substance Name	Pine oil

CAS No.	**8002-09-3**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Water
Estimated Distribution and Media Concentration	**0.469**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Pine oil
CAS No.	**8002-09-3**
Model Conditions	**25 °C,** 100,000 Ibs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Soil
Estimated Distribution and Media Concentration	**0.33**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Pine oil
CAS No.	**8002-09-3**
Model Conditions	**25** “C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Sediment
Estimated Distribution and Media Concentration	**0.0073**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Pine oil
CAS No.	**8002-09-3**
Model Conditions	**25 °C,** 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Suspended Sediment
Estimated Distribution and Media Concentration	**0.00023**
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.

References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Pine oil
CAS No.	8002-09-3
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Fish
Estimated Distribution and Media Concentration	0.000019
Data Qualities Reliabilities	Reliable with restriction.
Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Pine oil
CAS No.	8002-09-3
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated log Kow, water solubility, VP, MP
Media	Aerosol
Estimated Distribution and Media Concentration	0.0000025
Data Qualities Reliabilities	Reliable with restriction.

Data Reliability Remarks	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

3 Ecotoxicity

3.1 Acute Toxicity to Fish

Substance Name	2,6,6-Trimethylbicyclo[3.1 .1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)
CAS No.	125252-49-5
Method/guideline	Followed method n the OECD Guidelines for Testing Chemicals (1992) No. 203, " Fish Acute Toxicity Test" referenced as Method C.I of Commission Directive 92/69/EEC.
Test Type	Acute Fish Toxicity
GLP	Yes
Year	1997
Species/Strain/Supplier	Juvenile rainbow trout
Analytical Monitoring	Moving average method of Thompson
Exposure Period	96 hr
Remarks for Test Conditions	Based on the results of the range-finding study, the following test concentrations were assigned to the definite study: 1.5, 2.7, 4.8, 8.5 & 15 mg/l. Test material was dissolved in and controls were exposed to dimethylformamide.
Observations	8.5 mg/L: Highest concentration resulting in 0% mortality; 15 mg/L: lowest concentration resulting in 100% mortality; No observed effect concentration (NOEC): 2.7 mg/L; sub-lethal effects were observed at concentration of 4.8 mg/L and above.
Nominal Concentrations as mg/L	1.5, 2.7, 4.8, 8.5 & 15 mg/L
Measured Concentrations as mg/L	1.47, 2.55,4.53, 13.9 mg/l
Remarks for Results	Sub-lethal effects observed were increased pigmentation, swimming at the bottom of the test vessels with increased pigmentation, swimming at the surface with increased pigmentation and the presence of moribund fish.
Conclusion Remarks	The acute toxicity of the test material to the fresh water fish rainbow trout has been investigated and gave a 96-hr LC50 value of 11 mg/L with 95% confidence limit of 8.515 mg/l. No-Observed-Effect Concentration was 2.7 mg/L.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	The study was performed in compliance with U.K. GLP standard. These regulations are in accordance with GLP standards published as OECD monograph No. 45 (OECD/GD/(92)32) and are in conformity with, and implement, the requirement Directive 87/18/EEC.
Reference	Wetton P. M. (1997a). Plinyl Acetate: Acute Toxicity to Rainbow Trout (Oncohychus mykiss). Safepharm Laboratories Ltd. SPL Project Number: 10441012.

Substance Name	alpha-Terpineol (90% + 10% emulsifier
CAS No.	98-55-5
Method/guideline	Method used was in accordance with Protocol outlined by Wan et al. (1990, 1991) and by Environment Canada 91990a, 1990b)
Test Type	Acute Fish Toxicity
GLP	N G
Year	1998
Species/Strain/Supplier	Coho salmon and Rainbow trout
Exposure Period	96 hr
Remarks for Test Conditions	10 fishes were exposed to the test substance and observed for 24, 48, 72 and 96 hour. LC50 values were calculated using the "Lethal Computer Program" developed by Stephen (1977, revised in 1983)
Nominal Concentrations as mg/L	5 nominal concentration below 100 ppm were selected
Remarks for Results	LC50 for Coho Salmon =6.8 ppm; LC50 for Rainbow Trout = 6.7 ppm
Conclusion Remarks	The LC50 for Coho Salmon was determined to be 6.8 mg/l and for Rainbow Trout was 6.7 mg/l.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions
Data Reliability Remarks	Article was published in Bull. Environ. Contam. Toxicol.
Reference	Stroh J., Wan, M. T., Isman, M. B. and Moul, D. J. (1998) Evaluation of the acute toxicity to juvenile pacific coho salmon and rainbow trout of some plant essential oils, a formulated product, and the carrier. Bull Enviro. Contam. Toxicol. 60: 923-930

Substance Name	Myrcenol
CAS No.	**543-39-5**
Method/guideline	The test was conducted by EPA-ASTH procedure using 10 fathead minnows per test concentrations in a total volume of 10 liters. Temperature, fish survival, pH and dissolved oxygen levels were monitored during the test period of 96 hours.
Test Type	Acute Fish Toxicity
GLP	**NG**
Year	**1986**
Species/Strain/Supplier	Fathead minnows
Analytical Monitoring	Temperature, pH, fish survival and dissolved oxygen levels

Exposure Period	96 hr
Remarks for Test Conditions	Minimal aeration was supplied when the dissolved oxygen was below 4 mg/L. All samples were tested within six hours after the collection without pH adjustment or solids removal.
Observations	Median lethal concentration (LC50)=3.7 mg/L
Conclusion Remarks	Median lethal concentration (LC50)=3.7 mg/L
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Reference	UCC Business Confidential (1986). Ecological Fate and Effects Testing of UCC Products and Wastewaters During 1985. Unpublished Report.

Substance Name	Pine oil (62.7% alpha-terpineol, 83.4% total terpene alcohol content)
CAS No.	**8002-09-3**
Method/guideline	Bioassays were carried out according to the procedures outlined in APHA 1975. Standard Method for examination of water & waste water. APHA, American Water Works Association, Water Pollution Control Federation. 14th Ed. Wash. DC 1193p.
Test Type	Acute Fish Toxicity (range finding test)
GLP	N G
Year	1994
Species/Strain/Supplier	Juvenile Rainbow trout (Salma, gairdneri).
Exposure Period	96 hrs
Remarks for Test Conditions	Concentrations tested: 25, 50, 75, 100, 200 & 1000 mg/L. The percentage of survival of the fish in the solution was observed at 24, 48, 72 & 96 hours. LC50 values and their 95% confidence limits were calculated according to Stephan (1977).
Conclusion Remarks	96 hour LC50 was calculated to be 71 mg/L (95% CI=50-100)
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	The study was conducted in accordance with APHA procedure.
Reference	Graves, W. C. and Swigert, J. P (1994b). Pine Oil: 96-Hours Flow-through Acute Toxicity Test with the Rainbow Trout (Oncorhynchus mykiss). Wildlife International Ltd Report to The CSMA Pine Oil Joint Venture. Lab Project ID/Study Number 274A-102.

Substance Name	Pine oil Disinfectant (80:10:10) (mixture contains 50-60% alpha-terpineol and IO-I 5% terpineol isomers)
CAS No.	**8002-09-3**
Method/guideline	The procedure used was that described in the 1 Ith edition of Standard Methods for Examination of Waters and Waste

	Waters & the Sept 8, 1964 "Dept of Interior Guide for Evaluation of Wildlife.
Test Type	Acute Fish Toxicity
GLP	N G
Year	1965
Species/Strain/Supplier	Bluegill fingerlings (Lepomis macrochirus)
Exposure Period	24 & 48 hrs
Observations	LC50 at 24 h= 59 mg/L; LC50 at 48 h= 58 mg/L
Conclusion Remarks	The LC50 of the test material was calculated to be 58-59 mg/l
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliability Remarks	The study was conducted in accordance with Dept of Interior Guideline.
Reference	Ryckman, Edgerley, Burbank and Associates (1965) Investigation of treatability and fish toxicity of certain manufacturing products and wastes and their decay under stream conditions. Unpublished report to Hercules Powder Co.

Substance Name	The study was conducted using structurally related Iso-Linalool (2,4-Dimethyl 2,7-Octadien-4-ol).
CAS No.	78-70-6
Method/guideline	The protocol followed the standard procedures described in the EPA/OTS guidelines for testing the effects of chemicals on fish and meet the TSCA guidelines as specified in the appropriate Registration Standard.
Test Type	Acute Fish Toxicity
GLP	Yes
Year	1990
Species/Strain/Supplier	Rainbow trout (Oncorhynchus mykiss)
Analytical Monitoring	All samples analyzed by HPLC
Exposure Period	24, 48, 72 & 96 hours.
Nominal Concentrations as mg/L	100, 60, 36, 22 and 13 mg active ingredient/L
Measured Concentrations as mg/L	77, 44, 25, 17 and 10 mg active ingredient/L
Unit	Mg active ingredient/L
Remarks for Results	The 96-hour LC50 value was estimated by non-linear interpolation to be 33 mg/L; 95% confidence interval was calculated by binomial probability to be 25-44 mg/L. The No Observed Effect Concentration established for this study was 10 mg A.I./L.

Conclusion Remarks	The 96-hr LC50 value was estimated to 33 mg/L; 95% confidence interval was calculated to be 25-44 mg/L. The No Observed Effect Concentration established for this study was 10 mg A.I./L.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions,
Data Reliability Remarks	The study was conducted in accordance to GLP.
Reference	LeLievre, M. (1990a) 2,4-Dimethyl 2,7-octadien-4-ol)-acute toxicity to rainbow trout (Oncorhynchus mykiss) under static conditions. Springborn Lab. Inc. Report Submitted to SCM Glidco Organics. SLI Report # 90-g-3476.

Substance Name	Linalool
CAS No.	78-70-6
Method/guideline	EPA ECOSAR Model
Test Type	Acute Fish Toxicity
Exposure Period	96 hr
Observations	96 Hour LC50= 0.60 mg/l
Unit	mg/l
Reference	EPA ECOSAR

Substance Name	Myrcenol
CAS No.	**543-39-5**
Method/guideline	EPA ECOSAR
Test Type	Acute Fish Toxicity
Exposure Period	96 hr
Observations	96 Hour LC50 = 4.85 mg/l
Unit	mg/l
Reference	EPA ECOSAR

Substance Name	Dihydromyrcenol
CAS No.	**18479-58-8**
Method/guideline	EPA ECOSAR
Test Type	Acute Fish Toxicity

Exposure Period	96 hrs
Observations	96 Hour LC50 = 4.81 mg/l
Unit	mg/l
Reference	EPA ECOSAR

Substance Name	Linalyl acetate
CAS No.	115-95-7
Method/guideline	EPA ECOSAR
Test Type	Acute Fish Toxicity
Exposure Period	96 hrs
Observations	96 Hour LC50 = 4.9 mg/l using the calculated Kow of 3.46 but is 9.8 if you use the measured log Kow of 2.9
Unit	mg/l
Reference	EPA ECOSAR

Substance Name	Tetrahydrolinalool
CAS No.	**78-69-3**
Method/guideline	EPA ECOSAR
Test Type	Acute Fish Toxicity
Exposure Period	96 hr
Observations	96 Hour LC50 = 3.68 mg/l
Unit	mg/l
Reference	EPA ECOSAR

Substance Name	alpha-Terpineol
CAS No.	98-55-5
Method/guideline	EPA ECOSAR
Test Type	Acute Fish Toxicity
Exposure Period	**96** hrs
Observations	96 Hour LC50 = 13.7 mg/l

Unit	mg/l
Reference	EPA ECOSAR

Substance Name	alpha-Terpinyl acetate
CAS No.	80-26-2
Method/guideline	EPA ECOSAR
Test Type	Acute Fish Toxicity
Exposure Period	**96 hrs**
Observations	96 Hour LC50 = 1.75 mg/l based on log Kow = 4.3
Unit	mg/l
Reference	EPA ECOSAR

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)
CAS No.	125252-49-5
Method/guideline	EPA ECOSAR
Test Type	Acute Fish Toxicity
Exposure Period	96 hrs
Observations	**96 Hour LC50 = 17.4** mg/l
Unit	mg/l
Reference	EPA ECOSAR

Substance Name	*trans*-Pinanol
CAS No.	**4948-29-2**
Method/guideline	EPA ECOSAR
Test Type	Acute Fish Toxicity
Exposure Period	96 hrs
Observations	96 Hour LC50 = 18.2 mg/l
Unit	mg/l
Reference	EPA ECOSAR

Substance Name	cis-2-Pinanol
CAS No.	4948-28-l
Method/guideline	EPA ECOSAR
Test Type	Acute Fish Toxicity
Exposure Period	96 hrs
Observations	96 Hour LC50 = 18.2 mg/l
Unit	mg/l
Reference	EPA ECOSAR

Substance Name	Pinanol hydroperoxide
CAS No.	**28324-52-9**
Method/guideline	EPA **ECOSAR** – calculated as the decomposition product 2-pinanol)
Test Type	Acute Fish Toxicity
Exposure Period	96 hrs
Observations	96 Hour LC50 = 18.2 mg/l
Unit	mg/l
Reference	EPA ECOSAR

Substance Name	Pine oil
CAS No.	**8002-09-3**
Method/guideline	EPA ECOSAR
Test Type	Acute Fish Toxicity
Exposure Period	96 hr
Observations	96 Hour LC50 = 14 mg/l calculated as alpha-Terpineol
Unit	mg/l
Reference	EPA ECOSAR

Substance Name	Pine oil (62.7% alpha-terpineol, 83.4% total terpene alcohol content)

CAS No.	**8002-09-3**
Method/guideline	Bluegills were exposed to a geometric series of 5 test concentrations, solvent control, and a negative (well water) control. Two replicate test chambers were maintained in each treatment and control group, with 10 bluegills in each test chamber.
Test Type	Acute Fish Toxicity
GLP	Yes
Year	1994
Species/Strain/Supplier	Bluegill (Lepomis macrochirus)
Analytical Monitoring	Quantification of Pine oil in exposure solution was based upon the analysis of alpha terpineol.
Exposure Period	96 hrs
Remarks for Test Conditions	Nominal test concentrations were based upon the results of a range finding toxicity test.
Nominal Concentrations as mg/L	7.8, 13, 22, 36, and 60 mg/L
Measured Concentrations as mg/L	6.4, 11, 21, 36 and 58 mg/L
Remarks for Results	96-Hour LC50: 53 mg/L; 95% Confidence Limit: >36 mg/L; No mortality concentration: 36 mg/L. At 36 mg/L, all fish became lethargic after 72 hrs; at 58 mg/L, all fish became lethargic within 5 hrs; by termination, 65% of fish at 58 mg/L were dead.
Conclusion Remarks	The 96-hour LC50 value for bluegill exposed to Pine oil blend was 53 mg/L. At the 95% confidence level, the LC50 value is above 36 mg/L.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	The study was conducted to conform with Good Laboratory Practice standards published by EPA and OECD.
Reference	Graves W. C. and Swigert, J. P (1994a) Pine Oil: 96-Hours Flow-through Acute Toxicity Test with Bluegill (Lepomis macrochirus). Wildlife International Ltd Report to The CSMA Pine Oil Joint Venture. Lab Project ID/Study Number 274A-101

Substance Name	Pine oil (62.7% alpha-terpineol, 83.4% total terpene alcohol content)
CAS No.	**8002-09-3**
Method/guideline	Rainbow Trout were exposed to a geometric series of 5 test concentrations, solvent control, and a negative (well water) control. Two replicate test chambers were maintained in each treatment and control group, with 10 trout in each test chamber.
Test Type	Acute Fish Toxicity
GLP	**Yes**
Year	**1994**

Species/Strain/Supplier	Rainbow Trout (Oncorhynchus mykiss)
Analytical Monitoring	Measured concentrations of alpha-terpineol were used to calculate the concentration of Pine oil in solution.
Exposure Period	96 hrs
Remarks for Test Conditions	Nominal test concentrations were based upon the results of a range finding toxicity test. Observations were made approximately 3, 24, 48, 72 and 96 hours after test initiation.
Nominal Concentrations as mg/L	6.5, 11, 18, 30 and 50 mg/L
Measured Concentrations as mg/L	6.2, 10, 17, 28 and 48 mg/L
Remarks for Results	96-Hour LC50: 18 mg/L; 95% Confidence limits: 16 & 21 mg/L; No mortality concentration: 10 mg/L.
Conclusion Remarks	The 96-hour LC50 value for Rainbow Trout exposed to Pine Oil Blend was 18 mg/L. The 95% confidence limits were 16 & 21 mg/L and the slope of the concentration-response curve was 9.4. The 96-hrs no mortality concentration was 10 mg/L.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	The study was conducted to conform to GLP published by US EPA and OECD.
Reference	Graves, W. C. and Swigert, J. P (1994b) Pine Oil: 96-Hours Flow-through Acute Toxicity Test with the Rainbow Trout (Oncorhynchus mykiss). Wildlife International Ltd Report to The CSMA Pine Oil Joint Venture. Lab Project ID/Study Number 274A-102.

3.2 Acute Toxicity to Aquatic Invertebrates

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)
CAS No.	**125252-49-5**
Method/guideline	OECD guideline for testing of Chemicals (1984) No. 202, "Daphnia sp., Acute Immobilization test" referenced as Method C.2 of Commission Directive 92/69/EEC.
Test Type	Acute Immobilization Test
GLP	**Yes**
Year	1997
Species/Strain/Supplier	Daphnia magna
Test Details	Following a preliminary range-finding study, 20 daphnids were exposed to an aqueous dispersion of the test material at conc. of 0.15, 0.27, 0.48, 0.85, 1.5, 2.7, 4.8, 8.5, & 15 mg/l for 48 hrs under static test conditions.

Remarks for Test Conditions	The number of immobilized Daphnia were recorded after 24 and 48 hours.
Nominal Concentrations as mg/L	0.15, 0.27, 0.48, 0.85, 1.5, 2.7, 4.8, 8.5 & 15
Measured concentrations as mg/L	In excess of the required 80% of nominal conc.
EC50, EL50, LC50 at 24, 48 hours	48 hour EC50 = 7.0 mg/ml with 95% CI-6.3-7.6 mg/l.
Remarks for Results	The No Observed Effect Concentration was 4.8 mg/L
Conclusion Remarks	The acute toxicity of Plinyl acetate to Daphnia magna has been investigated and gave a 48-hours EC50 of 7.0 mg/l with 95% CI of 6.3-7.6 mg/l. The No Observed Effect Concentration at 48 hours was 4.8 mg/l.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	The study was in compliance with the UK Principles of Good Laboratory Practice. These Principles are in accordance with GLP standards published as OECD Environment Monograph No. 45 (OECD/GD(92)32).
Reference	Wetton P. M. (1997b) Plinyl Acetate: Acute Toxicity to Daphnia Magna. Safepharm Laboratories, Inc. SPL Project Number: 1044/013.

Substance Name	Myrcenol
CAS No.	**543-39-5**
Method/guideline	The test procedure closely followed those recommended by the EPA Committee on Methods for Toxicity Tests with Aquatic organisms except replicate concentrations were not routinely used.
Year	1985
Species/Strain/Supplier	Daphnia magna
Test Details	The young Daphnia were randomly added to the test solution. Dissolved oxygen and pH were determined initially and at 48 hours for all test concentration & controls. Mortalities were recorded at 24 & 48 hours.
EC50, EL50, LC50 at 24, 48 hours	LC50=36 mg/L at 48 hours
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	The study was conducted in accordance with EPA recommended method.
Reference	UCC Business Confidential (1986). Ecological Fate and Effects Testing of UCC Products and Wastewaters During 1985. Unpublished Report.

Substance Name	Linalool (data for structurally related substance, isolinalool (2,4-dimethyl-2,7-octadien-4-ol) clear liquid, 93.73% pure)
CAS No.	78-70-6

Method/guideline	The protocol followed the standard procedures described in the EPA/OTS guidelines for testing the effects of chemicals on daphnids, and meets the TSCA guidelines as specified in the appropriate Registration Standard.
GLP	Yes
Year	1990
Analytical Procedures	High pressure liquid chromatography (HPLC)
Species/Strain/Supplier	Daphnia pulex
Nominal Concentrations as mg/L	180, 110, 65, 40, 23, and 14 mg A.I./L
Measured concentrations as mg/L	110, 63, 37, 24, 14, and 9.3 mg A.I./L
Unit	mg active ingredient/L
EC50, EL50, LC50 at 24, 48 hours	EC50=47 mg/L (95% CI: 42-53) @ 48 h
Biological Observations	At 48 hour, 100% immobilization in 110 mg A.I./L; 90% and 15% immobilization at 63 & 37 mg A.I./L, respectively; sub lethal effects (lethargy) at 63, 37, & 24 mg/L; no immobilization at 24, 14 or 9.3 mg/L;
Control Response	Yes
Statistical Evaluations	EC50 value was calculated by probit analysis
Conclusion Remarks	The EC/50 was 68 (95% CI 37-l 10) and 47 (95% CI 42-53) mg active ingredient/L at 24 and 48 hours respectively.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	The study was conducted in accordance with GLP guidelines
Reference	LeLievre M. (1990b) 2,4-Dimethyl 2,7-Octadien-4-ol - Acute Toxicity to Daphnids (Daphnia pulex) under static conditions. Springborn Lab. Inc. Submitted to SCM Glidco Organics, Inc. SLI Report # 90-g-3494.

Substance Name	Pine oil blend (62.7% alpha-terpineol, 83.4% total terpene alcohol content)
CAS No.	**8002-09-3**
Method/guideline	Daphnids were exposed to a geometric series of 5 test concentrations, a solvent control, and a negative (well water) control. Two replicate test chambers were maintained in each treatment and control group, with 10 daphnids in each test chambers.
Test Type	Acute toxicity test with the Daphnia magna
GLP	**Yes**
Year	**1994**
Analytical Procedures	Measured concentrations of alpha terpineol were used to calculate the concentrations of Pine Oil Blend in the test

	solutions.
Species/Strain/Supplier	Daphnia magna
Test Details	Daphnids were impartially assigned to exposure chambers at test initiation. Observations of mortality and other clinical signs were made approximately 19, 24 and 48 hours after the initiation.
Remarks for Test Conditions	Cumulative percent mortality and immobility observed in the treatment groups were used to calculate EC50 values at 24 and 48 hours. The no observed effect concentration was determined by examination of the mortality and clinical observation data.
Nominal Concentrations as mg/L	3.9, 6.5, 11, 18 and 30 mg/L
Measured concentrations as mg/L	3.7, 7.3, 11, 17 and 28 mg/L
EC50, EL50, LC50 at 24, 48 hours	24 mg/L at 48 hours
Biological Observations	48-hour EC50 = 24mg/L; 95% confidence limits: 17 and 28 mg/L; No observed effect concentration: 11 mg/L.
Control Response	Yes
Statistical Evaluations	Binomial method
Conclusion Remarks	The 48-hour EC50 value for daphnids exposed to Pine oil blend was 24 mg/L. The 95% confidence limits were 17 and 28 mg/L. The 48-hr no observed effect concentration was 11 mg/L.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	The study was conducted to conform to GLP by the US EPA and OECD.
Reference	Graves, W. C. and Swigert, J. P (1994c) Pine Oil: 48 Hours Flow-Through Acute Toxicity Test with the Cladoceran (Daphnia magna). Wildlife International Ltd. Report to The CSMA Pine Oil Joint Venture. Lab Project ID/No. 274A-103.

Substance Name	cis-2-Pinanol
CAS No.	**4948-28-I**
Method/guideline	ECOSAR
Test Type	Calculated based on measured Kow
Species/Strain/Supplier	Daphnia magna
Test Details	48 hrs
Remarks for Results	LC50 = 20.64 mg/l
Data Reliability Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
Reference	ECOSAR

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Method/guideline	ECOSAR
Test Type	Calculated based on measured Kow
Species/Strain/Supplier	Daphnia magna
Test Details	48 hrs
Remarks for Results	LC50 = 15.72 mg/l
Data Reliability Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
Reference	ECOSAR

Substance Name	alpha-Terpineol acetate
CAS No.	80-26-2
Method/guideline	ECOSAR
Test Type	Calculated based on measured Kow
Species/Strain/Supplier	Daphnia magna
Test Details	48 hrs
Remarks for Results	LC50 = 1.16 mg/l
Data Reliability Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
Reference	ECOSAR

Substance Name	Dihydromyrcenol
CAS No.	**18479-58-8**
Method/guideline	ECOSAR
Test Type	Calculated based on measured Kow
Species/Strain/Supplier	Daphnia magna
Test Details	48 hrs
Remarks for Results	LC50 = 5.70 mg/l

Data Reliability Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
Reference	ECOSAR

Substance Name	Linalyl acetate
CAS No.	115-95-7
Method/guideline	ECOSAR
Test **Type**	Calculated based on measured Kow
Species/Strain/Supplier	Daphnia magna
Test Details	48 hrs
Remarks for Results	LC50 = 1.04 mg/l
Data Reliability Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
Reference	ECOSAR

Substance Name	Myrcenol
CAS No.	**543-39-5**
Method/guideline	ECOSAR
Test Type	Calculated based on measured Kow
Species/Strain/Supplier	Daphnia magna
Test Details	48 hrs
Remarks for Results	LC50 = 5.75 mg/l
Data Reliability Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
Reference	ECOSAR

Substance Name	Pinane hydroperoxide
CAS No.	28324-52-9
Method/guideline	ECOSAR
Test Type	Calculated based on measured Kow
Species/Strain/Supplier	Daphnia magna

Test Details	48 hrs
Remarks for Results	LC50 = 20.64 mg/l (calculated as 2-Pinanol
Data Reliability Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
Reference	ECOSAR

Substance Name	Tetrahydrolinalool
CAS No.	78-69-3
Method/guideline	ECOSAR
Test Type	Calculated based on measured Kow
Species/Strain/Supplier	Daphnia magna
Test Details	48 hrs
Remarks for Results	LC50 = 4.40 mg/l
Data Reliability Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
Reference	ECOSAR

3.3 Acute Toxicity to Aquatic Plants

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)
CAS No.	125252-49-5
Method/guideline	The method followed that described in the OECD Guidelines for Testing of Chemicals (1984) No. 201, "Alga, Growth Inhibition Test" referenced as Method C.3 of Commission Directive 92/69/EEC (which constitutes Annex V of Council directive 67/548/EEC).
Test Type	Algae Growth Inhibition test
GLP	**Yes**
Year	**1997**
Species/Strain/Supplier	Green Algal, Scenedesmus subspicatus
Exposure Period	72 hr
Analytical Monitoring	Mean cell density was measured spectrophotometrically at 665 nm.

Nominal Concentrations mg/L	15 mg/l
NOEC, LOEC or NOEL, LOEL	EC50>15 mg/l; NOEC>15 mg/l
Control Response	Yes
Statistical Evaluations	A student t-test was carried out on the AUC @ 72h.
Conclusion Remarks	The EC50 & the NOEC was greater than 15 mg/l
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	The study was performed in compliance with UK GLP standard. These regulations are in accordance with GLP standards published as OECD Monograph No. 45 (OCDE/GD(92)32).
Reference	Mead C. (1997a) Plinyl Acetate: Algal Inhibition Test. Safepharm Laboratories, ltd. SPL Project Number 10441014.

Substance Name	Linalool (data for structurally related isomer, iso-linalool (2,4-diemthyl 2,7-octadien-4-ol) 93.7% pure)
CAS No.	78-70-6
Test Type	Acute toxicity to green alga
GLP	Yes
Year	1990
Species/Strain/Supplier	Freshwater green alga (Selenastrum capricornutum.
Endpoint Value	Reduction in cell density after 24, 48, 72 and 96
Exposure Period	96 hr
Remarks for Test Conditions	Test conditions: 96-hours duration, 24-28 C, constant illumination (4,000-5,000 lux), shaking at 100 rpm.
Nominal Concentrations mg/L	32, 16, 8.0, 4.0, 2.0 and 1.0 mg/L
Measured concentrations as mg/L	28, 14, 6.9, 3.3, 1.6 and 0.82 mg/L
Unit	mg/L
NOEC, LOEC or NOEL, LOEL	NOEC = 3.3 mg/L
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Reference	Giddings J. (1990). (2,4-Dimethyl 2,7-octadien-4-ol)-acute toxicity to freshwater green alga (Selenastrum capriornutum) under static conditions. Springborn Lab. Inc. Report Submitted to SCM Glidco Organics. SLI Report #390-10-3497.

Substance Name	*cis*-2-Pinanol
CAS No.	4948-28-l

Method/guideline	Calculated
Test Type	ECOSAR
Species/Strain/Supplier	Green algae
Exposure Period	96 hr
NOEC, LOEC or NOEL, LOEL	EC50 = 13.55 mg/l
Conclusion Remarks	EC50 = 13.55 mg/l
Data Reliability Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
Reference	ECOSAR

Substance Name	alpha-Terpineol
CAS No.	98-55-5
Method/guideline	Calculated
Test Type	ECOSAR
Species/Strain/Supplier	Green algae
Exposure Period	96 hr
NOEC, LOEC or NOEL, LOEL	EC50 = 10.40 mg/l
Conclusion Remarks	EC50 = 10.40 mg/l
Data Reliability Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
Reference	ECOSAR

Substance Name	alpha-Terpineol acetate
CAS No.	80-26-2
Method/guideline	Calculated
Test Type	ECOSAR
Species/Strain/Supplier	Green algae
Exposure Period	96 hr
NOEC, LOEC or NOEL, LOEL	EC50 = 0.14 mg/l
Conclusion Remarks	EC50 = 0.14 mg/l

Data Reliability Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
Reference	ECOSAR

Substance Name	Dihydromyrcenol
CAS No.	**18479-58-8**
Method/guideline	Calculated
Test **Type**	ECOSAR
Species/Strain/Supplier	Green algae
Exposure Period	96 hr
NOEC, LOEC or NOEL, LOEL	EC50 = 3.88 mg/l
Conclusion Remarks	EC50 = 3.88 mg/l
Data Reliability Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
Reference	ECOSAR

Substance Name	Linalool
CAS No.	78-70-6
Method/guideline	Calculated
Test Type	ECOSAR
Species/Strain/Supplier	Green algae
Exposure Period	96 hr
NOEC, LOEC or NOEL, LOEL	EC50 = 3.93mg/l
Data Reliability Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
Reference	ECOSAR

Substance Name	Linalyl acetate
CAS No.	115-95-7
Method/guideline	Calculated
Test Type	ECOSAR

Species/Strain/Supplier	Green algae
Exposure Period	96 hr
NOEC, LOEC or NOEL, LOEL	EC50 = 0.14 81 mg/l [Using Kow = 2.9]
NOEC, LOEC or NOEL, LOEL	EC50 = 0.14 mg/l
Data Reliability Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
Reference	ECOSAR

Substance Name	Myrcenol
CAS No.	543-39-5
Method/guideline	Calculated
Test Type	ECOSAR
Species/Strain/Supplier	Green algae
Exposure Period	96 hr
NOEC, LOEC or NOEL, LOEL	EC50 = 3.91 mg/l
Conclusion Remarks	EC50 = 3.91 mg/l
Data Reliability Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
Reference	ECOSAR

Substance Name	Tetrahydrolinalool
CAS No.	78-69-3
Method/guideline	Calculated
Test Type	ECOSAR
Species/Strain/Supplier	Green algae
Exposure Period	96 hr
NOEC, LOEC or NOEL, LOEL	EC50 = 3.02 mg/l
Conclusion Remarks	EC50 = 3.02 mg/l
Data Reliability Remarks	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
Reference	ECOSAR

Substance Name	Linalool
CAS No.	78-70-6
Method/guideline	Plate Inhibition Assay [Ikawa, 1985]
Test Type	Algal Growth Inhibition Test
GLP	NA
Year	1992
Species/Strain/Supplier	Green algae/Chlorella pyrenoidosa
Exposure Period	48 hr
Analytical Monitoring	Net diameter of inhibition zone=Total diameter -disk diameter.
Remarks for Test Conditions	Plates under fluorescent light and zones of inhibition read after 2 days. Net diameter of inhibition was mean of three disks per plate run on 2 separate occasions. Lightening or total wipe out of color in yellow green Chlorella lawn.
Nominal Concentrations mg/L	10, 1, and 0.1 mg/ml in ethanol
Unit	mg/ml
NOEC, LOEC or NOEL, LOEL	NOEC = 1 mg/ml (1000 mg/L)
Biological Observations	Lightening of lawn color at 10 mg/ml concentration compared to controls
Control Response	Yes
Statistical Evaluations	None
Conclusion Remarks	NOEC = 1.0 mg/ml (1000 mg/L)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions
Data Reliability Remarks	Data was reported in a peer-reviewed journal.
General Remarks	Authors noted that stored samples produced effects. Newly purchased samples were inactive. Inhibition occurred through vapor phase and not through diffusion in agar medium.
Reference	Ikawa M., Mosley S., and Barbero B. (1992) Inhibitory effects of terpene alcohols and aldehydes on the growth of green alga Chlorella pyrenoidosa. Journal of Chemical Ecology 18(10): 1755-l 760.

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Method/guideline	Plate Inhibition Assay [Ikawa, 1985]

Test Type	Algal Growth Inhibition Test
GLP	NA
Year	1992
Species/Strain/Supplier	Green algae/Chlorella pyrenoidosa
Exposure Period	48 hr
Analytical Monitoring	Net diameter of inhibition zone=Total diameter -disk diameter.
Remarks for Test Conditions	Plates under fluorescent light and zones of inhibition read after 2 days. Net diameter of inhibition was mean of three disks per plate run on 2 separate occasions. Lightening or total wipe out of color in yellow green Chlorella lawn.
Nominal Concentrations mg/L	10, 1, and 0.1 mg/ml in ethanol
Unit	mg/ml
NOEC, LOEC or NOEL, LOEL	NOEC = 10 mg/ml (10,000 mg/L)
Biological Observations	No signs of inhibition of growth of Clorella p. at any concentration tested.
Control Response	Yes
Statistical Evaluations	None
Conclusion Remarks	No effects on growth of Chlorella pryenoidosa. NOEC = 10.0 mg/ml (10,000 mg/L)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions
Data Reliability Remarks	Data was reported in a peer-reviewed.
Reference	Ikawa M., Mosley S., and Barbero B. (1992) Inhibitory effects of terpene alcohols and aldehydes on the growth of green alga Chlorella pyrenoidosa. Journal of Chemical Ecology. 18(10): 1755-l 760.

4 Human Health Data

4.1 Acute Toxicity

Substance Name	cis-2-Pinanol
CAS No.	4948-28-I
Method/guideline	Acute dermal toxicity was determined in male and female New Zealand white rabbits.
Test Type	Acute Dermal LD50 study
GLP	NG
Year	1979
Species/strain	White New Zealand rabbit
Sex	Male and Female
# of animals per sex per dose	2M and IF
Route of Administration	Dermal
Remarks for Test Conditions	Two male and one female rabbit were intact and 1 male and 2 females were abraded. Material applied in a close batch test. Animals were observed at I, 3, 6, and 24 hours, daily for 14 days, All rats were given a complete necropsy.
Value LD50 or LC50 with confidence limits	Dermal LD50 = >5000 mg/kg
Number of deaths at each dose level	No deaths reported.
Remarks for Results	No remarkable necropsy findings.
Conclusion Remarks	Acute dermal LD50> 5000 mg/kg
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Palanker A. L. and Lewis C. A. (1979) Acute toxicity studies in rats and rabbits. Unpublished report to RIFM.

Substance Name	Linalool
CAS No.	**78-70-6**
Method/guideline	Acute dermal toxicity was determined in albino rabbits
Test Type	Acute Dermal LD50 study
GLP	**NG**
Year	1970

Species/strain	Albino rabbit
Sex	Not reported
# of animals per sex per dose	3
Route of Administration	Dermal
Remarks for Test Conditions	Material was applied to shaved abdomen of rabbits in 24-hour closed-patch test. Animals were observed for 7 days. On day 5, hematology and clinical chemistry were performed. On day 7, animals were sacrificed as and necropsied.
Value LD50 or LC50 with confidence limits	Dermal LD50 = 5610 mg/kg (95% C.I. 3580-8370 mg/kg)
Number of deaths at each dose level	013 at 2500 mglkg, 1/3 at 5000 mg/kg, 313 at 10,000 mglkg.
Remarks for Results	Symptomatology: depression
Conclusion Remarks	Dermal LD50 was determined to be 5610 mglkg.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Fogelman R.W. (1970) Acute dermal toxicity study in rabbits. Unpublished report to RIFM.

Substance Name	cis-2-Pinanol
CAS No.	4948-28-l
Method/guideline	Acute oral toxicity was determined in male and female Wistar albino rats
Test Type	Acute Oral LD50 study
GLP	**NG**
Year	1979
Species/strain	Wistar rat
Sex	Male and Female
# of animals per sex per dose	5
Vehicle	Corn oil
Route of Administration	Oral
Remarks for Test Conditions	Rats fasted for 18 hours were given the test material at 25% in corn oil. Animals were observed at 1, 3, 6, and 24 hours, daily for 14 days All rats were given a complete necropsy.
Value LD50 or LC50 with confidence limits	Oral LD50= 2050 mg/kg (95% C. I., 1630-2580 mglkg)
Number of deaths at each dose level	1260 mglkg, 215 female deaths; 2,000 mglkg, 2/5 male and 3/5 female deaths; 2520 mglkg, 2/5 male and 4/5 female deaths; 3140 mg/kg, 4/5 male and 3/5 female deaths
Remarks for Results	Depression in 1 male and 5 females at 2000 mglkg. Depression in 4 male and 5 females at 2520 mg/kg. Depression in all at

	3140 mg/kg. No remarkable necropsy findings
Conclusion Remarks	Acute oral LD50 =2050 mglkg
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Palanker A. L. and Lewis C. A. (1979) Acute toxicity studies in rats and rabbits. Unpublished report to RIFM.

Substance Name	Pine oil • Hercules Fortified Pine-Odor Disinfectant-transparent yellow liquid (6060% terpineol isomers, mainly alpha-terpineol)
CAS No.	8002-09-3
Method/guideline	Acute Oral toxicity study in rats The technique of Weil, Thompson and Thompson and Weil was employed.
Test Type	Acute Oral toxicity study
GLP	N G
Year	1976
Species/strain	Sprague-Dawley rats
Sex	Female
# of animals per sex per dose	4
Route of Administration	Oral
Remarks for Test Conditions	Doses tested: 1350, 4556, 6834, 10250 & 15380 mglkg
Value LD50 or LC50 with confidence limits	Acute LD50 = 10250 mglkg +/- 1.475 mg/kg
Number of deaths at each dose level	1350 mg/kg-0/4; 4556 mg/kg-0/4; 6834 mg/kg-1/4; 10250 mglkg-114 and 15380 mg/kg-4/4
Remarks for Results	At necropsy- red discolored lungs, gastritis and pale, discolored kidneys. In addition, mottled livers were noted in 2 rats. Examination of the survivors did not reveal any gross pathologic alterations.
Conclusion Remarks	The oral LD50 of Hercules Fortified Pine-Odor Disinfectant was calculated to be 10,250 mg/kg in female Sprague-Dawley rats, and the substance was considered to be practically nontoxic.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Johnson M. C. and Lewis, R.F. (1976) Report to Hercules Inc. on Acute Toxicity Studies with Hercules Fortified Pine-Odor Disinfectant by Industrial Bio-Test Laboratories inc. Project No. 76-05. June 8, 1976.

Substance Name	Dihydromyrcenol
CAS No.	**1847958-8**
Method/guideline	Acute oral toxicity was determined in rats

Test Type	Acute Oral LD50 study
GLP	NG
Year	1973
Species/strain	Wistar rat
Sex	Male
# of animals per sex per dose	10
Route of Administration	Oral
Remarks for Test Conditions	No other details given.
Value LD50 or LC50 with confidence limits	Oral LD50 = 3600 mg/kg (C. I., 30004200 mg/kg)
Number of deaths at each dose level	2560 mg/kg, 1/10 deaths; 3200 mg/kg, 5/10 deaths; 4000 mg/kg, 4/10 deaths; 5000 mglkg, 10110 deaths.
Remarks for Results	Lethargy occurred in all groups
Conclusion Remarks	Acute oral LD50 = 3600 mg/kg
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Moreno 0. M. (1973) Dihydromyrcenol. Acute toxicity studies in rats and rabbits. Unpublished report to RIFM.

Substance Name	Myrcenol
CAS No.	**543-39-5**
Method/guideline	Acute oral toxicity was determined in rats
Test Type	Acute Oral LD50 study
GLP	Ng
Year	1972
Species/strain	Wistar rat
Sex	Male
# of animals per sex per dose	10
Route of Administration	Oral
Remarks for Test Conditions	No other details given.
Value LD50 or LC50 with confidence limits	Oral LD50 = 5300 mglkg (C. I., 4500-6100 mglkg)
Number of deaths at each dose level	4000 mglkg, 2/10 deaths; 5,000 mg/kg, 4110 deaths; 6250 mglkg, 7/10 deaths; 7,800 mglkg, IO/IO deaths.
Conclusion Remarks	Acute LD50 study

Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Moreno 0. M. (1972b) Acute toxicity studies in rats and rabbits. Unpublished report to RIFM.

Substance Name	Hercules 70L Pine Oil Disinfectant, transparent yellow liquid
CAS No.	8002-09-3
Method/guideline	Acute oral Lethal Dose (LD50) was determined using the techniques of Weil, Thompson, and Thompson and Weil.
Test Type	Acute Oral Lethal Dose
GLP	NG
Year	1976
Species/strain	Albino Sprague Dawley rats
Sex	Female
# of animals per sex per dose	4
Route of Administration	Oral
Remarks for Test Conditions	Doses tested 1350, 2025, 3038, 4556, 15380 mglkg. All doses were administered directly into the stomachs of the rats using a hypodermic syringe equipped with a ball-tipped intubating needle.
Value LD50 or LC50 with confidence limits	Acute Oral LD50 = 4118 mglkg +/- 418.1 mglkg
Number of deaths at each dose level	At 1350 mg/kg-0/4; at 2025 mg/kg-0/4; at 3038 mglkg 0/4; at 4556 mg/kg-3/4, at 15380 mglkg-414.
Remarks for Results	No gross pathological alterations. Hemorrhage in stomach lining at 4556 mglkg; white mucoid substance in GI tract at 15380 mg/kg.
Conclusion Remarks	The acute oral LD50 value of Hercules 70L Pine oil Disinfectant in the female Sprague Dawley rats was calculated to be 4118 mglkg +/- 418.1 mg/kg. The substance was classified as slightly toxic.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Baker R. G., Mastri, C. W., Kinoshita, F. K and Keplinger, M. L. (1976) Report to Hercules Inc. on Acute Toxicity Studies with Hercules 70L Pine Oil Disinfectant by Industrial Bio-Test Laboratories, Inc. Project No. 76-05. Dated June 8, 1976.

Substance Name	Riser Pine oil (5060% alpha-terpineol, IO-I 5% other terpineol isomers, 7-15% terpene secondary alcohols and IO-20% terpene hydrocarbons)
CAS No.	**8002-09-3**
Method/guideline	Approximate Lethal Dose (A.L.D.) was studied by the Deichman and LaBlanc method.

Test Type	Approximate Lethal Dose Test
GLP	Pre GLP
Year	1961
Species/strain	Rats
Sex	Male and Female
# of animals per sex per dose	3
Route of Administration	Oral
Remarks for Test Conditions	Test material was administered undiluted by stomach tube in a single oral dose (ranging from 0.94 g/kg to 7.1 g/kg). The surviving animals were scarified after a period of 2 weeks. A post mortem examination was performed on each of the rats.
Value LD50 or LC50 with confidence limits	The Approximate Lethal Oral dose of Riser Pine oil in the **rat** was found to be 2.1 g/kg. This dose killed in 54 hours.
Number of deaths at each dose level	Dose 0.94 & 1.4 g/kg-survived; at 2.1 g/kg died in 54 hrs; at 3.2 g/kg died in 36 hrs; at 4.7 & 7.1 died in 12 hours.
Remarks for Results	Signs of intoxication: loss of equilibrium, decreased sensitivity to pain, increased salivation and muscular weakness, increased secretion of lacrimal fluid, occasional clonic convulsions, loss of body wt., hyperemic lungs, hemorrhagic atelectasis, etc.
Conclusion Remarks	The Approximate Lethal Oral dose of Riser Pine oil in the rat was found to be 2.1 g/kg. This dose killed in 54 hours.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Deichmann, W. B. (1961) Report on the Determination of the Approximate Lethal Oral Dose in the Rat of Compounds Submitted by the Hercules Powder Co.

Substance Name	Linalyl acetate
CAS No.	**115-95-7**
Method/guideline	Acute dermal toxicity in the rabbit
Test **Type**	Acute Dermal LD50 study
GLP	**NG**
Year	**1972**
Species/strain	Rabbit
Sex	Not reported
# of animals per sex per dose	3
Route of Administration	Dermal
Remarks for Test Conditions	No other details given.

Value LD50 or LC50 with confidence limits	Acute Dermal LD50 was determined to be greater than 5,000 mg/kg
Number of deaths at each dose level	No deaths at 5000 mg/kg dose.
Conclusion Remarks	Dermal LD50 was determined to be >5000 mg/kg.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Moreno 0. M. (1972a) Linalyl acetate. Acute toxicity studies in rats and rabbits. Unpublished report to RIFM.

Substance Name	Myrcenol
CAS No.	**543-39-5**
Method/guideline	Acute dermal toxicity in the rabbit
Test Type	Acute Dermal LD50 study
GLP	NG
Year	1972
Species/strain	White New Zealand rabbit
Sex	Not reported
# of animals per sex per dose	10
Route of Administration	Dermal
Remarks for Test Conditions	No other details given.
Value LD50 or LC50 with confidence limits	Acute dermal LD50 was determined to be greater than 5,000 mg/kg
Number of deaths at each dose level	No deaths at highest dose.
Conclusion Remarks	Dermal LD50 was determined to be >5,000 mg/kg.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Moreno 0. M. (1972b) Acute toxicity studies in rats and rabbits, Unpublished report to RIFM.

Substance Name	Dihydromyrcenol
CAS No.	18479-58-8
Method/guideline	Acute dermal toxicity in the rabbit
Test Type	Acute dermal LD50 study
GLP	**NG**
Year	1973

Species/strain	White New Zealand rabbit
Sex	Not reported
# of animals per sex per dose	10
Route of Administration	Dermal
Remarks for Test Conditions	No other details given.
Value LD50 or LC50 with confidence limits	Acute Dermal LD50 was determined to be greater than 5,000 mg/kg
Number of deaths at each dose level	No deaths at highest dose.
Conclusion Remarks	Dermal LD50 was determined to be >5000 mg/kg.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Moreno 0. M. (1973) Dihydromyrcenol. Acute toxicity studies in rats and rabbits. Unpublished report to RIFM.

Substance Name	2,6,6-Trimethylbicyclo[3.1 .1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)
CAS No.	**125252-49-5**
Method/guideline	The study was performed to assess the acute oral toxicity of Plinyl acetate in Sprague-Dawley CD strain rats. The method followed the OECD Guidelines for Testing of chemicals No 401 "Acute Oral Toxicity" and Method B1 of Commission Directive 92/69/EEC
Test Type	Acute Oral LD50
GLP	Yes
Year	1997
Species/strain	Sprague-Dawley CD Strain rats
Sex	Male and Female
# of animals per sex per dose	5
Route of Administration	Oral
Remarks for Test Conditions	5 male and 5 female rats were dosed (2000 mg/kg; dose volume 2.11 ml/kg) the animals were observed for deaths or overt signs of toxicity for 112, 1, 2 & 4 hours after dosing and subsequently once daily for 14 days.
Value LD50 or LC50 with confidence limits	>2000mg/kg
Number of deaths at each dose level	No deaths reported
Remarks for Results	There were no deaths or clinical signs of systemic toxicity. All animals showed an expected body weight gain and no abnormalities were noted at necropsy

Conclusion Remarks	The acute oral median lethal dose (LD50) of Plinyl acetate in the Sprague-Dawley CD strain rat was found to be greater than 2000mg/kg.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliabilities Remarks	Study was conducted in compliance with UK GLP and methodology recommended in the OECD Guidelines for testing of Chemicals No.401 "Acute Oral Toxicity" and Method B1 of Commission Directive 92/69/EEC.
References	Sanders A. (1997). Plinyl Acetate: Acute Oral Toxicity (Limit Test) in the Rats. Safepharm Laboratories Ltd. SPL Project No. 1044/004.

Substance Name	alpha-Terpineol acetate
CAS No.	80-26-2
Method/guideline	Litchfield-Wilcoxon, 1949 (FDA study)
Test Type	Acute Oral LD50 study
GLP	NG
Year	1964
Species/strain	Osborne-Mendel rat
Sex	Male and Female
# of animals per sex per dose	5
Route of Administration	Intubation
Remarks for Test Conditions	Five male and five female young adult Osborne-Mendel rats were fasted for 18 hours prior to treatment. Two weeks thereafter, animals were observed.
Value LD50 or LC50 with confidence limits	Oral LD50= 5075 mg/kg (C. I., 4160-6190 mg/kg)
Number of deaths at each dose level	Not given
Remarks for Results	Animals exhibited depression, scrawny appearance, and porphyrin-like deposits around eyes and nose
Conclusion Remarks	Oral LD50 was determined to be 5075 mg/kg for rats.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliabilities Remarks	Data appeared in peer-reviewed journal.
References	Jenner P. M., Hagan, E.C., Taylor, J.M., Cook, E.L. and Fitzhugh, O.G. (1964) Food Flavorings and Compounds of Related Structure I. Acute Oral Toxicity. Food and Cosmetics Toxicology 2:327-343.

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)

CAS No.	125252-49-5
Method/guideline	The method used test the Acute Inhalation Toxicity Potential of the Plinyl acetate followed the recommendation of the OECD Guidelines for Testing Chemicals No. 403 "Acute Inhalation Toxicity of Chemicals" and method B2 of Commission Directive 92/69/EEC.
Test Type	Acute Inhalation Toxicity
GLP	Yes
Year	1997
Species/strain	Sprague-Dawley CD rats
Sex	Male and Female
# of animals per sex per dose	5
Route of Administration	Inhalation (nose only)
Remarks for Test Conditions	Each rat was individually held in a tapered polycarbonate restraining tube fitted onto a single tier of the exposure chamber. Only the nose of each animal was exposed (5 mg/l) to the test atmosphere for 4 hours
Value LD50 or LC50 with confidence limits	LC50 > 5.03 mg/l
Number of deaths at each dose level	Not given
Remarks for Results	No deaths, wet fur, hunched posture and pilo-erection, occasional labored &/or noisy respiration, ptosis, tiptoe gait and red/brown staining of the fur and around the eyes snout and head was observed. Dark areas or dark foci on the lungs were seen.
Conclusion Remarks	The acute inhalation median lethal concentration of the Plinyl acetate in the Sprague-Dawley CD rat was > 5.03 mg/l.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliabilities Remarks	Study was performed in compliance with UK GLP standard. These regulations are also in accordance with GLP standards published by OECD monograph No. 45 (OCDE/GD(92)32).
References	Blagden S. M. (1997). Plinyl Acetate: Acute Inhalation Toxicity (Nose Only) Study in the Rat. Safepharm Laboratories Ltd. SPL Project No. 10441017.

Substance Name	Linalool
CAS No.	**78-70-6**
Method/guideline	Litchfield-Wilcoxon, 1949 (FDA study)
Test Type	Acute Oral LD50 study
GLP	**NG**
Year	1964

Species/strain	Osborne-Mendel rat
Sex	Male and Female
# of animals per sex per dose	5
Route of Administration	Intubation
Remarks for Test Conditions	Five male and five female young adult Osborne-Mendel rats were fasted for 18 hours prior to treatment. Two weeks thereafter, animals were observed.
Value LD50 or LC50 with confidence limits	**Oral** LD50 = 2790 mg/kg (C. I., 2440-3180 mg/kg)
Number of deaths at each dose level	**Not** given
Remarks for Results	Animals expired between 4 and 18 hours after dose.
Conclusion Remarks	Oral LD50 was determined to be 2790 mg/kg for rats.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliabilities Remarks	Data appeared in peer-reviewed journal.
References	Jenner, P.M., Hagan, E.C.,Taylor, J.M, Cook, E.L. and Fitzhugh, O.G. (1964). Food Flavorings and Compounds of Related Structure I. Acute Oral Toxicity. Food and Cosmetics Toxicology 2:327-343.

Substance Name	Tetrahydrolinalool
CAS No.	78-69-3
Method/guideline	Acute oral toxicity was determined in rats
Test Type	Acute LD50 study
GLP	NG
Year	1976
Species/strain	Rats
Sex	Not reported
# of animals per sex per dose	10
Route of Administration	Oral
Remarks for Test Conditions	No other details given.
Value LD50 or LC50 with confidence limits	Oral LD50 was found to be greater than 5.0 g/kg
Number of deaths at each dose level	Not given
Remarks for Results	Symptomatology: lethargy

Conclusion Remarks	Oral LD50 was found to be greater than 5.0 g/kg
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Moreno O.M. (1976) Acute toxicity studies in rats, mice, rabbits and guinea pigs. Unpublished report to RIFM.

Substance Name	Tetrahydrolinalool
CAS No.	78-69-3
Method/guideline	Acute Dermal Toxicity in rabbit was determined.
Test Type	Acute Dermal LD50 study
GLP	NG
Year	**1976**
Species/strain	Rabbits
Sex	Not reported
# of animals per sex per dose	10
Route of Administration	Dermal
Remarks for Test Conditions	No other details given
Value LD50 or LC50 with confidence limits	Dermal LD50 was found to be greater than 5 g/kg
Number of deaths at each dose level	Not given
Remarks for Results	9/10 animals had moderate redness and moderate edema. 1/10 had slight redness and slight edema.
Conclusion Remarks	Dermal LD50 was found to be greater than 5 g/kg
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Moreno 0. M. (1976) Acute toxicity studies in rats, mice, rabbits and guinea pigs. Unpublished report to RIFM.

Substance Name	Linalyl acetate
CAS No.	115-95-7
Method/guideline	Litchfield-Wilcoxon, 1949 (FDA study)
Test Type	Acute Oral LD50 study
GLP	**NG**
Year	164
Species/strain	Osborne-Mendel rat

Sex	Male and Female
# of animals per sex per dose	5
Route of Administration	Intubation
Remarks for Test Conditions	Five male and five female young adult Osborne-Mendel rats were fasted for 18 hours prior to treatment. Two weeks thereafter, animals were observed.
Value LD50 or LC50 with confidence limits	Oral LD50= 14,550 mg/kg (C. I., 12,300-17,170 mg/kg)
Number of deaths at each dose level	Not given
Remarks for Results	Animals showed depression soon after treatment, coma and wet posterior.
Conclusion Remarks	Oral LD50 was determined to be 14,550 mg/kg for rats.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliabilities Remarks	Data appeared in peer-reviewed journal.
References	Jenner P.M., Hagan, EC., Taylor, J.M. Cook, E.L. and Fitzhugh, O.G. (1964) Food Flavorings and Compounds of Related Structure I. Acute Oral Toxicity. Food and Cosmetics Toxicology 2:327-343.

Substance Name	Tetrahydrolinalool
Test Type	Acute Dermal Toxicity study
GLP	NG
Year	1976
Species/strain	Rabbits
Sex	Not reported
# of animals per sex per dose	10
Route of Administration	Dermal
Value LD50 or LC50 with confidence limits	Acute Dermal LD50 was determined to be greater than 5.00 g/kg
Number of deaths at each dose level	Not given
Remarks for Results	Moderate redness and edema was noted in 9 out of 10 rabbits. Slight redness and edema was noted in one rabbit.
Conclusion Remarks	Acute dermal LD50 of tetrahydrolinalool was determined to be greater than 5.00 glkg
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Moreno. 0. M. (1976). Report to RIFM by M.B. Research Laboratories, Inc.

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Method/guideline	Acute oral toxicity was determined in male Cd-I mice.
Test Type	Acute Oral LD50 study
GLP	NG
Year	1985
Species/strain	CD-I mouse
Sex	Male
# of animals per sex per dose	10
Route of Administration	Oral
Remarks for Test Conditions	Animals were assessed for 7 days post-treatment,
Value LD50 or LC50 with confidence limits	Oral LD50 = 2830 mglkg (95% C. I., 2290-3497 mglkg)
Number of deaths at each dose level	Not given
Conclusion Remarks	Oral LD50 = 2830 mglkg
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Yamahara J., Kimura H., Kobayashi M., Okamoto T., Sawada T., Fujimura H., and Chistaka T. (1985) Cholagogic action and characteristics of (+/-)-alpha-terpineol-beta-D-O-glucopyranoside, a new monoterpenoid glucoside. Chem. and Pharm. Bulletin. 33(4) 1669.

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Method/guideline	Approximate Lethal Dose (A.L.D.) was studied by the Deichman and LaBlanc method.
Test Type	Approximate Lethal Dose Test
GLP	**NG**
Year	**1961**
Species/strain	Rats
Sex	Not reported
Route of Administration	Oral
Remarks for Test Conditions	Test material was administered undiluted by stomach tube in a single oral dose. The surviving animals were scarified after a period of 2 wks. Post mortem examination were performed.

Value LD50 or LC50 with confidence limits	The Approximate Lethal Oral dose of alpha-Terpineol in the rat was found to be 3.2 g/kg.
Number of deaths at each dose level	Not given
Conclusion Remarks	The Approximate Lethal Oral dose of alpha-Terpineol in the rat was found to be 3.2 g/kg.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Deichmann W. B. (1961) Report on the determination of the approximate lethal oral dose in the rat of compounds. Submitted by the Hercules Powder Co.

Substance Name	20% Pine Oil disinfectant (pine oil contained 76.7% alpha- and gamma-terpineol)
CAS No.	8002-09-3
Method/guideline	The study was designed to comply with the standards set forth by EPA proposed Guidelines for Test Procedures (1982), Subsection F. Series 81-1.
Test Type	Acute Oral toxicity study
GLP	Yes
Year	1985
Species/strain	Wistar Albino rats
Sex	Male and Female
# of animals per sex per dose	5
Route of Administration	Oral
Remarks for Test Conditions	5 male & 5 female rats were dosed by gavage with 20% Pine oil disinfectant in water at 5.0 g/kg and observed for 1, 2, & 4 hrs post dose and twice daily for 14 days.
Value LD50 or LC50 with confidence limits	LD50 was calculated to be greater than 5.0 g/kg (LD50>1g/kg for pine oil undiluted.).
Number of deaths at each dose level	Not given
Remarks for Results	Symptoms: Lethargy, ataxia, piloerection, chromorhinorrhea, chromodacryorrhea, pstois and brown staining of anogenital area. Body weight /necropsy normal.
Conclusion Remarks	According to EPA criteria, 20% Pine oil Disinfectant was considered to be Category IV.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliabilities Remarks	Study was conducted in accordance with the GLP regulations of the FDA effective 06/20/79 and EPA effective 11/29/83.
References	Cerven B., Moreno, 0. M. and Althenbach, E. (1985a) Single Dose Oral Toxicity in Rats (20% Pine Oil Disinfectant. Report to Hercules Inc. by M. B. Research Laboratories. Project No. MB 85-7546 A.

Substance Name	20% Pine Oil Disinfectant, Pale Yellow Liquid (pine oil contained 76.7% alpha- and gamma-terpineol)
CAS No.	8002-09-3
Method/guideline	The study was designed to comply with the standards set forth by EPA proposed Guidelines for Test Procedures (1982), subsection F. Series 81-2.
Test Type	Acute Dermal LD50 study
GLP	Yes
Year	1985
Species/strain	Albino New Zealand rabbits
Sex	Male and Female
# of animals per sex per dose	5
Route of Administration	Dermal
Remarks for Test Conditions	2.0 g/kg of the test material was applied to the shaved dermal sites on the back of health rabbits (5 per sex). The test material was kept in contact with the skin for 24 hours. Dermal responses were recorded on day 1, 7, and 14.
Value LD50 or LC50 with confidence limits	The Dermal LD50 was determined to be greater than 2.0 g/kg (LD50>0.4 g/kg as pine oil undiluted.)
Number of deaths at each dose level	Not given
Remarks for Results	Dermal reaction was moderate on day 1, severe on Day 7 and absent to slight on Day 14. An instance of diarrhea decreased fecal output and yellow nasal discharge were noted.
Conclusion Remarks	The Dermal LD50 was determined to be greater than 2.0 g/kg. According to EPA criteria, 20% Pine oil disinfectant was considered to be Category III.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliabilities Remarks	Study was conducted in accordance with the GLP regulations of the FDA effective 06/20/79 and EPA effective 1 1/29/83.
References	Cerven B., Moreno, 0. M. and Althenbach, E. (1985b). Acute Dermal Toxicity in Rabbits (20% Pine Oil Disinfectant. Report to Hercules Inc. by M. B. Research Laboratories. Project No. MB 85-7546 B.

Substance Name	Hercules 70L Pine Oil Disinfectant, transparent yellow liquid
CAS No.	**8002-09-3**
Method/guideline	Acute dermal Lethal Dose (LD50) was determined using the techniques of Weil, Thompson, and Thompson and Weil.
Test Type	Acute Dermal Toxicity
GLP	Ng
Year	1976

Species/strain	White New Zealand rabbits
Sex	Male
# of animals per sex per dose	4
Route of Administration	Dermal
Remarks for Test Conditions	Test material (3000 mg/kg) was applied to the shaved area on the back of rabbits and occluded for 24 hrs. After 24 hrs, test material was removed and animals were observed for local skin reactions for 14 days.
Value LD50 or LC50 with confidence limits	The Dermal LD50 value was calculated to be greater than 3000 mg/kg.
Number of deaths at each dose level	Not given
Remarks for Results	Severely irritating to the skin of rabbits, beet red erythema, severe edema and 2nd degree bum. Escharosis was observed at the test skin sites at 7 & 14 days. Hemorrhaged lungs and gastroenteritis was also seen in one rabbit each.
Conclusion Remarks	The Dermal LD50 value for Hercules 70L Pine Oil Disinfectant was calculated to be greater than 3000 mg/kg. The test material was considered to be practically nontoxic.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Baker R. G., Mastri, C. W., Kinoshita, F. K and Keplinger, M. L. (1976) Report to Hercules Inc. on Acute Toxicity Studies with Hercules 70L Pine Oil Disinfectant by Industrial Bio-Test Laboratories, Inc. Project No. 76-05. Dated June 8, 1976.

Substance Name	Pine Oil (100%), clear liquid (62.7% alpha-terpineol, 83.4% total terpene alcohol content)
CAS No.	8002-09-3
Method/guideline	The test material was tested for acute inhalation toxicity in conformity with the EPA Guidelines. Five male and five female rats (Sprague-Dawley) were exposed for 4 hours to dynamic atmosphere containing a nominal concentration of 9.2-mg/L air.
Test Type	Acute Inhalation toxicity
GLP	**Yes**
Year	1994
Species/strain	Sprague Dawley rat
Sex	Male and Female
# of animals per sex per dose	5
Route of Administration	Inhalation
Remarks for Test Conditions	The actual concentration measured in the breathing zone thrice during the exposure was 3.98 mg/l, 3.92 mg/l and 3.48 mg/l.
Value LD50 or LC50 with confidence limits	The LC50 > 3.79 mg/L.

Number of deaths at each dose level	Not given
Remarks for Results	After exposure, all rats appeared wet and common signs were depressed activity, yellow abdominal and perineal staining (urine), and frequent chromorhinorrhea, one female showed ataxia and also had nasal discharge.
Conclusion Remarks	The LC50 was greater than 3.79 mg/L. The EPA toxicity indicator for Pine oil is best described as Category III/IV, No morality at 3.79 mg/L.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliabilities Remarks	Study was conducted in accordance with EPA Guidelines.
References	Robbins G. R. (1994) Acute Inhalation Toxicity Study in Rats. Pine Oil. Cosmopolitan Safety Evaluation, Inc. Report to CSMA Pine Oil Joint Venture. Lab Project ID/Study Number C3371.

4.2 Genetic Toxicity *In* Vitro

Substance Name	Linalyl acetate
CAS No.	**115-95-7**
Method/guideline	Linalyl acetate was tested in the rat hepatocytes for unscheduled DNA synthesis
Test Type	Unscheduled DNA Synthesis
System of Testing	Rat hepatocytes
GLP	NG
Year	1989
Species/Strain	Sprague-Dawley or Fischer Rat
Metabolic Activation	None
Doses/Concentration	300 ug
Remarks for Test Conditions	The Hepatocytes were isolated from adult male rats and incubated for 18-20 hours with the test material in serum-free WME medium containing 5-10uCi/ml 3h-TdR. UDS was measured by electronically counting nuclear grains and subtracting the average number of grains in 3 adjacent nuclear-sized cytoplasmic areas.
Results	Linalyl acetate gave a negative response.
Genotoxic effects	None
Conclusion Remarks	Linalyl acetate was not shown to be clastogenic under the test conditions.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.

Remarks for Data Reliability	The study was published in a peer-reviewed journal The Toxicologist.
References	Heck J.D., Vollmuth, T.A., Cifone, M.A, Jagannath, D.R., Myhr, B. and Curren, R.D. (1989) An Evaluation of Food Flavoring Ingredients in a Genetic Toxicity Screening. The Toxicologist Vol 9 NO. 1.

Substance Name	Linalool
CAS No.	78-70-6
Method/guideline	The Mouse Lymphoma L5178y TK +/- cell Mutagenesis (MLY) assay was performed according to the procedures described by Clive et al. (1979).
Test Type	Mouse Lymphoma Forward Mutation Assay (MLY).
System of Testing	L5178y Mouse Lymphoma cell line
GLP	N G
Year	1989
Species/Strain	Mice
Metabolic Activation	Aeroclor 1254-induced rat liver S-9 activation system.
Doses/Concentration	3.9 nl/ml -200 nl/ml +S-9: 3.9150 nl/ml, -S-9
Results	Linalool was weakly positive in the presence of rat liver S-9 activation system.
Remarks for Results	At concentration range of 100 - 300 nl/ml linalool treatment resulted in 2.3-4.1 fold increase.
Conclusion Remarks	Linalool was weakly positive in the absence of rat liver S-9 activation system. However, these finding should be viewed with caution in light of the known effect of nonphysiological medium conditions on the outcome of such assays.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The study was published in a peer-reviewed journal The Toxicologist.
References	Heck J.D., Vollmuth, T.A., Cifone, M.A., Jagannath, D.R., Myhr, B. and Curren, R.D. (1989) An Evaluation of Food Flavoring Ingredients in a Genetic Toxicity Screening. The Toxicologist Vol 9 NO. 1.

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)
CAS No.	125252-49-5
Method/guideline	Ames
Test Type	Reverse mutation
System of Testing	Bacterial

GLP	Yes
Year	1997
Species/Strain	Salmonella typhimurium TA 100, TA 98, TA 1535, TA 1537 & TA 1538.
Metabolic Activation	Rat liver microsome fraction S9 from Aroclor induced rats.
Doses/Concentration	5 -5000 microliters per plate.
Statistical Methods	All data were analyzed by method recommended by the UKEMS and normally Dunnett's method of linear regression was used.
Remarks for Test Conditions	After 48-hour incubation at 37 °C, each assay plate was counted. Routine positive control plates were prepared: N-ethyl-N'nitro-N-nitrosoguanidine for TA100 & TA1535; 9-Aminoacridine for TA1537; 4-Nitro-o-phenylenediamine for TA 98; 4-Nitroquinoline-1-oxide for TA98 & 2-Aminoanthracene which is non-mutagenic in the absence of S9 was used.
Results	No biologically significant increase in revertant colonies was observed with any bacterial strains and any dose of the test material either with or without metabolic activation.
Cytotoxic concentration	500 ug/plate
Genotoxic effects	None
Statistical results	N G
Remarks for Results	A slight increase in revertant colonies was observed with tester strain TA98 with metabolic activation only, but the response did not achieve a 2-fold increase over the concurrent solvent controls and non-reproducible in three experiments, of which included a pre-incubation method and a tightened test material doserange.
Conclusion Remarks	No evidence of mutagenicity.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions. Data were acquired prior to GLP or OECD guidelines but were obtained by standard methodology and published in a peer reviewed journal.
Remarks for Data Reliability	The study was performed in compliance with UK GLP standard and is in accordance with GLP standards published as OECD Monograph No. 45 (OCDE/GD(92)32).
References	Thompson P. W. (1997) Plinyl Acetate: Reverse Mutation Assay "Ames Test" Using Salmonella Typhimurium. Safepharm Laboratories Ltd. SPL Project Number 1044/010.

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance • plinyl acetate, clear colorless non-viscous liquid)
CAS No.	**125252-49-5**
Method/guideline	The method used followed that described in the OECD Guidelines for testing Chemicals (1981) No. 473 "Genetic toxicology: Chromosome Aberration Test" and Method B10 of Commission Directive 92/69/EEC.

Test Type	Chromosomal Aberration
System of Testing	In vitro human lymphocytes
GLP	Yes
Year	1997
Species/Strain	Human volunteer whole blood
Metabolic Activation	S9 Fraction prepared from male rat liver treated with single (500 mg/kg, ip) Aroclor 1254 injection
Doses/Concentration	15.31, 30.63, 61.25, 122.5, 245, 490, 980, & 1960 ug/ml
Statistical Methods	Frequency of cells with aberration and frequency of polyploid was compared with the concurrent vehicle control using Fischer's Exact test or Chi-squared test.
Remarks for Test Conditions	Four treatment conditions were used in 4 hrs exposures with the addition of S9 from rat liver at 10% in standard cofactors with cell harvest after 16 & 40 hr expression periods and a 20 & 44 hr continuous exposure in the absence of activation. In experiment 1 the dose range for evaluation was selected from series of 8 dose levels on the basis of toxicity.
Results	All vehicle controls gave frequencies of cells with aberration within the range expected for normal human lymphocytes. All the positive control treatments gave significant increases in the frequency of cells with aberration indicating the satisfactory performance of the test and of the activity of the metabolizing system.
Conclusion Remarks	Plinyl acetate was shown to be non-clastogenic to human lymphocytes in vitro, in presence or absence of liver enzyme metabolizing system.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The study was performed in compliance with UK GLP standard and is in accordance with GLP standards published as OECD Monograph No. 45 (OCDE/GD(92)32).
References	Wright N. P. (1997) Plinyl Acetate: chromosome aberration test in human lymphocytes in vitro. Safepharm Laboratories Ltd. SPL Project No. 1044101 1.

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Method/guideline	Test material was assayed for mutagenicity toward Salmonella typhimurium (TA 98, TA 100, TA 1535, & TA 1537) in the presence or absence of Liver S9 fraction from Aroclor 1250 treated Sprague-Dawley rats
Test Type	Reverse mutation (Ames test)
System of Testing	Bacterial
GLP	**NG**

Year	**1980**
Species/Strain	Bacteria; Salmonella typhimurium Strain TA98, TA1 00, TA1 535 & TA1537
Metabolic Activation	Liver S9 fraction from Aroclor 1250 treated Sprague-Dawley rats
Doses/Concentration	0.03, 0.3, 3.0 & 30.0 umol/plate.
Results	alpha-Terpineol was not found to be mutagenic.
Cytotoxic concentration	NA
Genotoxic effects	None
Conclusion Remarks	alpha-Terpineol was not found to be mutagenic.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The study was published in a peer-reviewed journal The Toxicologist.
References	Florin I., Rutberg, L, Curvall, M, and Enzell, C. R. (1980) Screening of Tobacco Smoke Constituents for Mutagenicity Using the Ames' Test. Toxicology, 18, 219-232.

Substance Name	Linalool
CAS No.	***78-70-6***
Method/guideline	Reverse mutation assays using S. *typhimurium* strains: TA92, TA1535, TA 100, TA 1537 & TA 98 were used according to the method of Ames, The S-9 was prepared from the Fischer rat liver treated with polychlorinated biphenyl (500 mg/kg).
Test Type	Reverse mutation (Ames test)
System of Testing	Bacterial
GLP	NG
Year	1984
Species/Strain	Bacteria: ***Salmonella typhimurium*** strains: TA92, TA1 535, TA 100, TA 1537 & TA 98
Metabolic Activation	The S-9 was prepared from the Fischer rat liver treated with polychlorinated biphenyl (500 mglkg).
Doses/Concentration	Maximum concentration 1 .0 mg/plate
Remarks for Test Conditions	The number of revertant (his+) colonies was scored after incubation at 37 C for 2 days. Vehicle: DMSO.
Results	No significant increase in the number of revertant colonies was observed at maximum concentration.
Cytotoxic concentration	NG
Genotoxic effects	No genotoxic effect
Conclusion Remarks	No genotoxic effects of Linalool were observed at maximum concentration of 1 .0 mg/plate in Reverse mutation assay (Ames Test)

Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The study was published in a peer-reviewed journal Food. Chem. Toxic.
References	Ishidate M, Sofuni, K., Yoshikawa, M., Nohmi, T., Sawada, M and Matsuoka, A. (1984) Primary Mutagenicity Screening of Food Additives Currently Used in Japan. FD. Chem. Tox. 22(8), 623-636.

Substance Name	Linalool
CAS No.	78-70-6
Method/guideline	Chromosomal Aberration test was carried out using a Chinese hamster fibroblast cell line. The cells were exposed to Linalool at three different concentrations for 24 & 48 hrs. No metabolic activation system was applied.
Test Type	Chromosomal Aberration test
System of Testing	Chinese hamster fibroblast cell line
GLP	N G
Year	1984
Species/Strain	Hamster: Chinese hamster fibroblast cell line.
Remarks for Test Conditions	The incidence of polyploid cells as well as of structural chromosomal aberrations such as chromatid or chromosomal gaps, breaks, exchanges, ring formation, fragmentations and others, was recorded on each plate. Solvent treated/untreated cells served as negative control. Vehicle: DMSO
Results	Negative chromosomal test.
Statistical results	Results negative if the incidence was < 4.9%
Remarks for Results	The incidence of polyploid cells as well as of structural chromosomal aberrations such as chromatid or chromosomal gaps, breaks, exchanges, ring formation, fragmentations and others was less than 4.9%.
Conclusion Remarks	Linalool is not considered to be clastogenic under the test conditions.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The study was published in a peer-reviewed journal Fd. Chem. Toxic.
References	Ishidate M, Sofuni, K., Yoshikawa, M., Nohmi, T., Sawada, M and Matsuoka, A. (1984) Primary Mutagenicity Screening of Food Additives Currently Used in Japan. FD. Chem. Tox. 22(8), 623-636.

Substance Name	Linalool
CAS No.	78-70-6

Method/guideline	Mutagenic effects of Linalool was tested in 5 tester strains of Salmonella typhimurium TA 1535, TA 1537, TA1538, TA 98 & TA 100 in the presence or absence of S-9 fraction of aroclor 1254 induced male Sprague-Dawley rat liver.
Test Type	Reverse mutation (Ames test)
System of Testing	Bacterial
GLP	NG
Year	1989
Species/Strain	Bacteria: Salmonella typhimurium TA 1535, TA 1537, TA1538, TA 98 & TA 100
Metabolic Activation	S-9 fraction of Aroclor 1254 induced male Sprague-Dawley rat liver.
Doses/Concentration	10,000 ug/plate
Results	Linalooi was inactive in Salmonella strains TA 1535, TA 1537, TA 1538, TA 98 & TA 100 both in the presence and absence of metabolic activation system.
Genotoxic effects	No genotoxic effect
Conclusion Remarks	Linalool was not found to be mutagenic in Reverse mutation assay (Ames' test) under the condition of this study.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The study was published in a peer-reviewed journal The Toxicologist.
References	Heck J.D., Vollmuth, T.A., Cifone, M.A., Jagannath, D.R., Myhr, B. and Curren, R.D. (1989) An Evaluation of Food Flavoring Ingredients in a Genetic Toxicity Screening. The Toxicologist Vo19N0.1.

Substance Name	Linalyl acetate
CAS No.	115-95-7
Method/guideline	Mutagenic effects of Linalyl acetate was tested in 5 tester strains of Salmonella typhimurium TA 1535, TA 1537, TA1538, TA 98 & TA 100 in the presence or absence of S-9 fraction of Aroclor 1254 induced male Sprague-Dawley rat liver.
Test **Type**	Reverse mutation (Ames test)
System of Testing	Bacterial
GLP	**NG**
Year	**1989**
Species/Strain	Bacteria: Salmonella typhimurium TA 1535, TA 1537, TA1538, TA 98 & TA 100
Metabolic Activation	S-9 fraction of Aroclor 1254 induced male Sprague-Dawley rat liver.
Doses/Concentration	25,000 ug/plate

Results	Linalyl acetate was inactive in Salmonella strains TA 1535, TA 1537, TA 1538, TA 98 & TA 100 both in the presence and absence of metabolic activation system.
Genotoxic effects	No genotoxic effect
Conclusion Remarks	Linalyl acetate was not found to be mutagenic under the test condition.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The study was published in a peer-reviewed journal The Toxicologist.
References	Heck J.D., Vollmuth, T.A., Cifone, M.A., Jagannath, D.R., Myhr, B. and Curren, R.D. (1989) An Evaluation of Food Flavoring Ingredients in a Genetic Toxicity Screening. The Toxicologist Vol 9 NO. 1.

Substance Name	Linalool
CAS No.	78-70-6
Method/guideline	Linalool was tested in the rat hepatocytes for unscheduled DNA synthesis
Test Type	Unscheduled DNA Synthesis
System of Testing	Rat hepatocytes
GLP	**NG**
Year	1989
Species/Strain	Sprague-Dawley Rat or Fischer Rat
Metabolic Activation	None
Doses/Concentration	**5oug**
Remarks for Test Conditions	The Hepatocytes were isolated from adult male rats and incubated for 18-20 hours with the test material in serum-free WME medium containing 5-10uCi/ml 3h-TdR. UDS was measured by electronically counting nuclear grains and subtracting the average number of grains in 3 adjacent nuclear-sized cytoplasmic areas.
Results	Linalool gave a negative response.
Genotoxic effects	None
Conclusion Remarks	Linalool was not shown to be clastogenic under the test conditions.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The study was published in a peer-reviewed journal The Toxicologist.
References	Heck J.D., Vollmuth, T.A., Cifone, M.A., Jagannath, D.R., Myhr, B. and Curren, R.D. (1989) An Evaluation of Food Flavoring Ingredients in a Genetic Toxicity Screening. The Toxicologist Vol 9 NO. 1.

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Method/guideline	The Mouse Lymphoma L5178y TK +/- cell Mutagenesis (MLY) assay was performed according to the procedures described by Clive et al. (1979).
Test Type	Mouse Lymphoma Forward Mutation Assay (MLY).
System of Testing	L5178y Mouse Lymphoma cell line
GLP	N G
Year	1989
Species/Strain	Mice
Metabolic Activation	Aroclor 1254-induced rat liver S-9 activation system.
Doses/Concentration	250-300 nl/ml
Results	alpha-Terpineol was found to be negative in the presence or absence of rat liver S-9 activation system.
Conclusion Remarks	alpha-terpineol was found to be negative in the presence or absence of rat liver S-9 activation system.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The study was published in a peer-reviewed journal.
References	Heck J.D., Vollmuth, T.A., Cifone, M.A., Jagannath, D.R., Myhr, B. and Curren, R.D. (1989) An Evaluation of Food Flavoring Ingredients in a Genetic Toxicity Screening. The Toxicologist Vol 9 NO. 1.

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Method/guideline	Mutagenic effects of alpha terpineol was tested in 5 tester strains of Salmonella typhimurium TA 1535, TA 1537, TA1538, TA 98 & TA 100 in the presence or absence of S-9 fraction of Aroclor 1254 induced male Sprague-Dawley rat liver.
Test Type	Reverse mutation (Ames test)
System of Testing	Bacterial
GLP	**NG**
Year	1989
Species/Strain	Bacteria: Salmonella typhimurium TA 1535, TA 1537, TA1538, TA 98 & TA 100
Metabolic Activation	S-9 fraction of Aroclor 1254 induced male Sprague-Dawley rat liver.

Doses/Concentration	10,000 ug/plate
Results	alpha-Terpineol was inactive in Salmonella strains TA 1535, TA 1537, TA 1538, TA 98 & TA 100 both in the presence and absence of metabolic activation system.
Genotoxic effects	No genotoxic effect
Conclusion Remarks	alpha-Terpineol was not found to be mutagenic under the test condition
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The study was published in a peer-reviewed journal.
References	Heck J.D., Vollmuth, T.A., Cifone, M.A., Jagannath, D.R., Myhr, B. and Curren, R.D. (1989) An Evaluation of Food Flavoring Ingredients in a Genetic Toxicity Screening. The Toxicologist Vol 9 NO. 1.

Substance Name	Linalool
CAS No.	78-70-6
Method/guideline	Mutagenic effects of linalool were tested in Salmonella typhimurium TA 98 & TA 100 in the presence or absence of S-9 fraction from rat liver.
Test Type	Reverse mutation (Ames test)
System of Testing	Bacterial
GLP	NG
Year	1979
Species/Strain	Bacteria: Salmonella typhimurium TA 98 & TA 100
Metabolic Activation	S-9 fraction from rat liver.
Remarks for Test Conditions	Rats were fed linalool and the ether extract and aqueous phase of 24-hour urine was assayed for mutagenicity. Direct urine samples were assayed with TA 100 and TA 98 either in the presence or absence of betaglucuronidase.
Results	No significant mutagenic activity was detected in either the ether phase or aqueous phase of urine.
Conclusion Remarks	Urine from linalool fed rats was shown to be non mutagenic.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions
References	Rockwell P. and Raw, I. (1979) A mutagenic screening of various herbs, spices, and food additives. Nutrition and Cancer I(4): 10-15.

Substance Name	Linalool
CAS No.	78-70-6

Method/guideline	0.5 ml of Linalool was administered directly through a gastric tube to 2 rats. Urine was collected on ice for 24 hr period.
Test Type	Reverse mutation (Ames test)
System of Testing	Bacterial
GLP	NG
Year	1979
Species/Strain	Bacteria: Salmonella typhimurium TA 98 & TA 100 & Sprague-Dawley rats
Metabolic Activation	Urine hydrolysis with beta-glucuronidase
Doses/Concentration	172 mg/kg
Remarks for Test Conditions	A screen for mutagenic activity was performed with the direct urine sample, either urine extract or the aqueous fraction. Assay was conducted with Salmonella typhimurium strain TA98 and TA1 00
Results	No mutagenic activity was detected when the direct urine samples or aqueous fraction were assayed either in presence or absence of beta-glucuronidase. Author had previously tested linalool and found it to be negative.
Genotoxic effects	None
Conclusion Remarks	No mutagenic activity was detected in the urine from rats given Linalool orally.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The study was published in a peer-reviewed journal.
References	Rockwell P. and Raw, I. (1979) A Mutagenic Screening of Various Herbs, Spices, and Food Additives. Nutrition and Cancer I: 10-15.

Substance Name	Linalool (substance tested was isomer, isolinalool, colorless liquid)
CAS No.	**78-70-6**
Method/guideline	Ames test: This method conforms to the guidelines for bacterial mutagenicity testing published by OECD. OECD Guidelines for Testing of Chemicals No. 471 “Reverse Mutation Study,” Method B14 of Common Directive 92/69/EEC.
Test Type	Reverse mutation
System of Testing	Bacterial
GLP	**Yes**
Year	**1999**
Species/Strain	Salmonella typhimurium strains TA1535, TA1537, TA98 and TA100; E. coli WP2uvrA-
Metabolic Activation	Rat liver homogenate

Doses/Concentration	15-5000 uglplate
Statistical Methods	Dunnett's method of linear regression
Remarks for Test Conditions	Salmonella typhimurium strains TA1 535, TA1 537, TA98 and TAIOO and E. coli WP2uvrA-were treated with test material using the Ames plate incorporation method at up to 6 dose levels, in triplicate, both with and without the addition of a rat liver homogenate metabolizing system. The vehicle DMSO) control plates gave counts of revertant colonies within the normal range
Results	Resulted in visible reduction in the growth of the bacterial lawn in all tester strains at 5000 uglplate; statistically significant increases in revertant colony frequency were observed in tester strains TA100 & TA1535 (without S9 mix only).; statistically significant increases & clear doserelated response in TA1535 with biggest increases at 3000 uglplate.
Cytotoxic concentration	5000 ug/plate
Remarks for Results	The test material was considered to be mutagenic under the conditions of the test.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The study was conducted in accordance with GLP.
References	LeLievre, M. (1990a) 2,CDimethyl 2,7-octadien-4-ol)-acute toxicity to rainbow trout (Oncorhynchus mykiss) under static conditions. Springborn Lab. Inc. Report Submitted to SCM Glidco Organics. SLI Report # 90-g-3476.

Substance Name	alpha-Terpineol
CAS No.	**98-55-5**
Method/guideline	Test substance was assayed for mutagenicity toward 4 histidine-requiring mutants of Salmonella typhimurium (TA98, TAIOO, TA1535 and TA1537). It was tested qualitatively both with and without metabolic activation using a liver fraction (S-9).
Test Type	Reverse mutation assay
System of Testing	Bacterial
GLP	**NG**
Year	**1980**
Species/Strain	Salmonella typhimurium (TA98, TAIOO, TA1535 and TA1537)
Metabolic Activation	Liver microsomal fraction from aroclor treated rats.
Doses/Concentration	3 umol/plate
Results	No mutagenic activity was detected.
Genotoxic effects	None

Conclusion Remarks	The test material was found to be non mutagenic under the test conditions
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions,
Remarks for Data Reliability	The study was published in a peer-reviewed journal.
References	Florin I., Rutberg, L., Curvall, M., and Enzell, CR. (1980) Screening of tobacco smoke constituents for mutagenicity using the Ames test. Toxicology 18: 219-232.

Substance Name	Pine oil blend, clear colorless liquid (76.7% alpha- and *gamma*-terpineol)
CAS No.	**8002-09-3**
Method/guideline	Unscheduled DNA synthesis was carried out using rat primary hepatocytes.
Test Type	Unscheduled DNA synthesis
System of Testing	Primary Rat hepatocytes
GLP	Yes
Year	1987
Species/Strain	Male Sprague Dawley rats
Doses/Concentration	Test article was tested at ten dose levels ranging from 0.0003 to 10 ul/ml and was fully evaluated at 5 dose levels of 0.0003, 0.001, 0.003, 0.01 and 0.03 in the initial assay.
Statistical Methods	Method of Casciano and Gaylor (Mutat Res 122: 81-86, 1983) were used.
Remarks for Test Conditions	Primary rat hepatocytes derived from the liver of adult male Sprague-Dawley rats were used in this study. The test article was dissolved and diluted in DMSO to make up the stock solution. The positive control cpd, 7,12-dimethylbenzanthracene, was also dissolved in DMSO. All test article and control treatments were done under subdued yellow lights to avoid possible problems of photoinactivation. In addition to above mentioned doses, 9 dose levels were tested in the confirmatory assay ranging from 0.0001 to 1 .O ul/ml and the same 5 concentrations to test article were fully evaluated.
Cytotoxic concentration	3.0 and 10 ul/ml
Genotoxic effects	None
Statistical results	Under the test conditions, the test article did not cause a significant increase in the Unscheduled DNA synthesis as measured by the mean number of net nuclear grain count at any dose level.
Conclusion Remarks	Pine oil blend is considered negative in Unscheduled DNA synthesis test
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The protocol of this study was designed to comply with all EPA, FDA and OECD test guidelines. This study was also performed in accordance with GLP guidelines.

References	Curren R. D. (1987) Unscheduled DNA Synthesis in Rat Primary Hepatocytes with a Confirmatory Assay. Microbiological Associate, Inc. Report to Chemical Specialties Manufacturers Association, Lab. Study No. T5366.380016.

Substance Name	Pine oil blend, clear colorless liquid
CAS No.	8002-09-3
Method/guideline	The test article was tested in the CHO/HGPRT mutation assay in the absence and presence of an Aroclor-induced rat liver S-9 activation system.
Test Type	CHO/HGPRT MUTATION ASSAY
System of Testing	CHO-K1-BH4 cells
GLP	Yes
Year	1987
Species/Strain	Chinese hamster ovary cells
Metabolic Activation	Aroclor induced male Fischer rat liver S-9 activation system.
Doses/Concentration	The first and the confirmatory assays were conducted at dose levels of 250, 200, 170, 130 and 100 nl/ml in the non-activated study and at 400, 300, 200, 100 and 50 nl/ml in the presence of s-9.
Remarks for Test Conditions	Ethyl methanesulfonate was used as positive control.
Results	The mutant frequencies of the test article treated groups were not increased significantly above the control, whereas EMS, positive control, induced a total of 180 mutants to yield mutant frequency of 271 .1mutants/10E6 clonable cells.
Genotoxic effects	None
Conclusion Remarks	Under the conditions of the assays, Pine Oil Blend was negative in the CHO/HPRT mutation assay.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The protocol of this study was designed to comply with all EPA, FDA and OECD test guidelines. This study was also performed in accordance with GLP guidelines.
References	Yang L. L. (1987) CHO/HGPRT Mutation Assay. Pine Oil Blend. Microbiological Associates Inc Report to Chemical Specialties Manufacturers Association. Lab. Study No. T5366.332001.

Substance Name	Tetrahydrolinalool 1
CAS No.	**78-69-3**
Method/guideline	Ames test was performed on five tester strains of Salmonella typhimurium (TA 1535, TA 100, TA 1537, TA 1538, TA 98.
Test Type	Reverse Mutation

System of Testing	Bacterial
GLP	NG
Year	1983
Species/Strain	Salmonella typhimurium (TA 1535, TA 100, TA 1537, TA 1538, TA 98.
Metabolic Activation	S-9 liver fraction was prepared from Aroclor-pretreated rats (Aroclor 1254, 500 mg/kg, ip).
Doses/Concentration	Up to 3600 ug/plate
Statistical Methods	Statistical significance was determined according to the methods of Kastenbaum and Bowman (1970).
Remarks for Test Conditions	Positive controls were run in each experiment with the reference mutagens sodium azide and benzo[a]pyrene.
Results	No mutagenic activity was detected with any of the Salmonella strains tested.
Cytotoxic concentration	NG
Genotoxic effects	None
Conclusion Remarks	No mutagenic activity was detected with any of the Salmonella strains tested.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The study was published in a peer-reviewed.
References	Wild D., King, M. T., Gocke, E. and Eckhardt. (1983). Study of Artificial Flavouring Substances for Mutagenicity in the Salmonella/Microsome, BASC and Micronucleus tests, Food and Chemical Toxicology 21(6), 707-719.

Substance Name	Linalool
CAS No.	78-70-6
Method/guideline	Ret-assay and mutation test
Test Type	Reverse Mutation
System of Testing	Bacterial
GLP	NG
Year	1986
Species/Strain	Bacteria: E.Coli WP2 uvrA
Metabolic Activation	None
Doses/Concentration	125-1000 ug/plate
Remarks for Test Conditions	Positive for reverse mutation if maximum revertants/spontaneous revertants>2.0.
Results	No mutagenic activity at any dose level.

Cytotoxic concentration	>1000 ug/plate
Genotoxic effects	None
Conclusion Remarks	No mutagenic effects in E. Coli.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Yoo Y.S. (1986) Mutagenic and antimutagenic activities of flavoring agents used in foodstuffs. Journal of the Osaka City Medical Center 34, 267-288

Substance Name	Linalool
CAS No.	78-70-6
Method/guideline	The DNA-repair test with Bacillus subtilis was performed as described by Kada et al. (1980).
Test Type	DNA-Repair test
System of Testing	Bacterial
GLP	N G
Year	1978
Species/Strain	Bacillus subtilis H17 Rec+ or M45 Rec-
Metabolic Activation	S9 fraction was prepared from the PCB-treated male Sprague-Dawley rats.
Doses/Concentration	17 ugldisk
Statistical Methods	N G
Results	No difference in zones of inhibition for H17 and M45.
Genotoxic effects	None
Statistical results	N G
Conclusion Remarks	No evidence of mutagenicity was detected under the test conditions.
Data Qualities Reliabilities	Reliability code 3. Data not reliable. Data in Japanese (not translated).
References	Oda Y., Hamono Y., Inoue K., Yamamoto H., Niihara T., and Kunita N. (1978) Mutagenicity of food flavors in bacteria. Shokuhin Eisei Hen 9, 177-181.

Substance Name	Linalool
CAS No.	78-70-6
Method/guideline	Spore plate rec assay
Test Type	DNA-Repair test

System of Testing	Bacterial
GLP	NG
Year	1986
Species/Strain	Bacillus subtilis H17 Rec+ or M45 Rec-
Metabolic Activation	S9 fraction was prepared from the PCB-treated male Sprague-Dawley rats.
Doses/Concentration	10 ug/disk
Statistical Methods	NG
Results	No difference in zones of inhibition for H17 and M45.
Genotoxic effects	None
Statistical results	NG
Conclusion Remarks	Mutagenicity at 10 nl/disk.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Yoo Y.S. (1986) Mutagenic and antimutagenic activities of flavoring agents used in foodstuffs. Journal of the Osaka City Medical Center 34, 267-288.

Substance Name	Linalool
CAS No.	*78-70-6*
Method/guideline	In vitro and In vivo-in vitro Mutagenicity Assay
Test Type	In vivo-in vitro Ames assay
GLP	NG
Year	1979
Species/Strain	Sprague-Dawley rats
Sex	Not given
Route of Administration	Oral gavage
Doses/Concentration	500 ul/rat (approximately 452 mg/rat)
Exposure Period	Urine collected over 24 hrs
Remarks for test conditions	In the in vitro assay, 0.05 to 100 ul/plate of linalool was incubated with strain TA 98 and TA 100 of *Salmonella typh.* with S-9 prepared from Aroclor 1254-treated rats. In the *in vivo-in* vitro experiment, rats (2) were given a 0.5 ml (452 mg) oral dose of linalool by oral intubation and the urine was collected over the next 24 hours. Fifty (50) to 300 ul of ether extracts of the urine, the aqueous fraction of the ether extracts, or un-extracted (direct) urine samples were then incubated with

	strains TA 98 and TA 100 for 48 hours. The direct urine mutagenicity assays were performed either in the presence of absence of *beta*-glucuronidase. Positive controls were sodium azide and picrolinic acid for TAIOO and TA98, respectively.
Genotoxic effects	None
NOEL (C)/ LOEL (C)	452 mglkg
Statistical Evaluation	A positive response in TAIOO was defined as any deviation above the upper limit of 99.9% confidence limits of the mean control values.
Remarks for Results	A standard Ames assay with Salmonella typhimurium strain TA98 and TAIOO was performed with the linalool in the presence of S-9, direct urine sample in the presence or absence of beta-glucuronidase, urine ether extract, or the aqueous fractions of ether extracts without S-9 activation.
Conclusion Remarks	There was no evidence of mutagenicity for linalool or linalool urinary metabolites in rats given 452 mg of linalool.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	Study was reported in Journal of Cancer and Nutrition.
References	Rockwell P. and Raw, I. (1979) A mutagenic screening of various herbs, spices, in food additives. Nutrition and Cancer I: IO-15

Substance Name	Linalyl acetate
CAS No.	115-95-7
Method/guideline	The DNA-repair test with Bacillus subtilis was performed as described by Kada et al. (1980).
Test Type	DNA-Repair test
System of Testing	Bacterial
GLP	**NG**
Year	1978
Species/Strain	Bacillus subtilis H17 Rec+ or M45 Rec-
Metabolic Activation	S9 fraction was prepared from the PCB-treated male Sprague-Dawley rats.
Doses/Concentration	18 ug/disk
Statistical Methods	**NG**
Results	No difference in zones of inhibition for H17 and M45.
Genotoxic effects	None
Statistical results	**NG**
Conclusion Remarks	No evidence of mutagenicity was detected under the test conditions.

Data Qualities Reliabilities	Reliability code 3. Data not reliable. Data in Japanese (not translated).
References	Oda Y., Hamono Y., Inoue K., Yamamoto H., Niihara T., and Kunita N. (1978) Mutagenicity of food flavors in bacteria. Shokuhin Eisei Hen 9, 177-181.

Substance Name	alpha-Terpineol acetate
CAS No.	80-26-2
Method/guideline	The DNA-repair test with Bacillus subtilis was performed as described by Kada et al. (1980).
Test Type	DNA-Repair test
System of Testing	Bacterial
GLP	NG
Year	1978
Species/Strain	Bacillus subtilis HI 7 Rec+ or M45 Rec-
Metabolic Activation	S9 fraction was prepared from the PCB-treated male Sprague-Dawley rats.
Doses/Concentration	19 ug/disk
Statistical Methods	NG
Results	No difference in zones of inhibition for H17 and M45.
Genotoxic effects	None
Statistical results	NG
Conclusion Remarks	No evidence of mutagenicity was detected under the test conditions.
Data Qualities Reliabilities	Reliability code 3. Data not reliable. Data in Japanese (not translated).
References	Oda Y., Hamono Y., Inoue K., Yamamoto H., Niihara T., and Kunita N. (1978) Mutagenicity of food flavors in bacteria. Shokuhin Eisei Hen 9, 177-181.

4.3 Genetic Toxicity *In* Vivo

Substance Name	Pine Oil Blend, clear, colorless liquid (76.7% alpha-and gamma-terpineol)
CAS No.	**8002-09-3**
Method/guideline	Mice were exposed to test article by single IP injection. The high dose **was** selected to represent 80% of the LD50/7. Bone marrow polychromatic erythrocytes were collected 24, 48 and 72 hours after the treatment. Bone Marrow polychromatic

	erythrocytes were hen examined microscopically for micronuclei.
Test Type	Micronucleus Cy-togenetic Assay
GLP	Yes
Year	1987
Species/Strain	Male and female CD-I mice
Sex	Male and female
Route of Administration	Intraperitoneal
Doses/Concentration	1155, 578, 116 mg/kg
Exposure Period	24, 48 and 72 hrs
Genotoxic effects	None
NOEL (C)/ LOEL (C)	1155 mg/kg
Statistical Evaluation	Kastenbaum-Bowman tables
Remarks for Results	The number of micronucleated erythrocytes was not significantly increased in test article treated groups, regardless of sex or sacrifice time point. TEM induced a significant increase in micronucleated polychromatic erythrocytes in male and female mice relative to the vehicle control.
Conclusion Remarks	Under the conditions of the assay, Pine Oil Blend didn't increase the incidence of micronucleated polychromatic erythrocytes in bone marrow and was concluded to be negative in the micronucleus test using male and female CD-I mice.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The study was performed in accordance with FDA GLP regulation, EPA GLPs and OECD guidelines.
References	Putman D. L. (1987) Micronucleus Cytogenetic Assay in Mice. Pine oil Blend. Microbiological Associates, Inc. Report to Chemical Specialties Manufacturers Association. Lab. Study Number T5366.122.

4.4 Repeat Dose Toxicity

Substance Name	alpha-Terpinyl acetate
CAS No.	80-26-2
Method/guideline	Method used by U.S. Food and Drug Administration.
GLP	P re-GLP
Year	1967

Species/strain	Osborne-Mendel rats
Sex	Male and Female
Route of Administration	Diet
Doses/concentration Levels	1000, 2500 *or* 10000 ppm
Exposure Period	20 weeks
Frequency of Treatment	Continuously in diet
Control Group	**Yes**
Post Exposure Observation Period	**NG**
Remarks for Test Conditions	Groups of ten male and ten female Osborne-Mendel rats were provided alpha-terpinyl acetate in the diet at concentrations of 0, 1000, 2500 or 10,000 ppm for 20 weeks. No vehicle was used. The diet was prepared and analyzed weekly. Measurements of body weight, food intake and general condition were recorded weekly. Hematological examinations (white cell counts, red cell counts, hemoglobin and hematocrit) were performed at the termination of the study. Macroscopic examination of all tissues was performed. Histopathological examination was performed on the liver, kidneys, spleen, heart, and testes of. 6-8 animals (evenly divided by sex) from the high dose and controls.
NOAEL (NOEL)	10000 ppm
LOAEL (LOEL)	No adverse effects at highest dose
Actual Dose Received by Dose Level and Sex	**NG**
Toxic Response/effects by Dose Level	None
Statistical Evaluation	**NG**
Remarks for Results	Determination of the dietary concentration of alpha-terpinyl acetate revealed a weekly loss of 7%. Measurements of body weight, food intake and general condition recorded weekly showed no significant differences between test and control animals at any intake level. At termination, hematological examinations revealed no difference from controls. At necropsy, no differences were reported between major organ weights of test and control animals. Gross examination of tissue of all animals was unremarkable and histopathological examination revealed no treatment-related lesions.
Conclusion Remarks	This study demonstrates a NOAEL in rats of at least 10,000 ppm
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions. This study was performed by the FDA prior to establishment of GLP & OECD.
References	Hagan E.C., Hansen W.H., Fitzhugh O.G., Jenner P.M., Jones W.I., Taylor J.M., Long E.L., Nelson A.A., and Brouwer J.B. (1967) Food Flavourings and Compounds of Related Structure. II. Subacute and Chronic Toxicity. Food Cosm Toxicology, 5, 141-157.

Substance Name	Linalool
CAS No.	78-70-6
Method/guideline	A rapid screening protocol incorporating key elements of the US NTP's immunotoxicity tier testing strategy was used to evaluate the effect of the test substance on humoral and cell-mediated immune responses.
GLP	NG
Year	1994
Species/strain	Mice: B6C3F1 mice
Sex	Female
Route of Administration	Intragastric
Doses/concentration Levels	375, 188 & 94 mglkglday in methyl cellulose
Exposure Period	5 days
Frequency of Treatment	Daily
Control Group	1% Methyl cellulose
Post Exposure Observation Period	10 days
Remarks for Test Conditions	Test material was administered intragastrically on a daily basis for 5 days at 3 dose levels to B6C3F1 mice. A host-resistance assay (Listeria monocytogenes bacterial challenge) was conducted to assess cell-mediate immunity. Humoral immunity was measured by the antibody Plaque-Forming cell (PFC) response to sheep erythrocytes. Cyclophosphamide served as an immunosuppressive positive control agent.
NOAEL (NOEL)	375 mglkglday
LOAEL (LOEL)	No adverse effects at highest dose
Toxic Response/effects by Dose Level	None
Remarks for Results	No increase in the mortality or significant alteration to the Plaque-Forming cell response was noted
Conclusion Remarks	Linalool did not mediate the cell-mediated or humoral immune response.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Gaworsky CL., Vollmuth, T.A., Dozier, M.M., Heck, J.D., Dunn, L.T., Ratajczak, H.V. and Thomas, P.T. (1994) An-Immunotoxicity Assessment of Food Flavouring Ingredients. Fd Chem. Toxic 32(5), 409415.

Substance Name	Linalyl acetate

CAS No.	115-95-7
Method/guideline	A rapid screening protocol incorporating key elements of the US NTP's immunotoxicity tier testing strategy was used to evaluate the effect of the test substance on humoral and cell-mediated immune responses.
GLP	N G
Year	1994
Species/strain	Mice: CD1 mice
Sex	Female
Route of Administration	Intragastric
Doses/concentration Levels	3000, 1500, 750 mg/kg/day in corn oil
Exposure Period	5 days
Frequency of Treatment	Daily
Control Group	Corn oil
Post Exposure Observation Period	10 days
Remarks for Test Conditions	Test material was administered intragastrically on a daily basis for 5 days at 3 dose levels to B6C3F1 mice. A host-resistance assay (Listeria monocytogenes bacterial challenge) was conducted to assess cell-mediate immunity. Humoral immunity was measured by the antibody Plaque-Forming cell (PFC) response to sheep erythrocytes. Cyclophosphamide served as an immunosuppressive positive control agent.
LOAEL (LOEL)	750 mglkglday
Toxic Response/effects by Dose Level	Increased mortality following challenge with L. monocytogenes was noted at 750 mg/kg. No significant alteration in the PFC response was noted.
Remarks for Results	The increased mortality observed following challenge with L. monocytogenes was not doserelated and therefore considered to be incidental.
Conclusion Remarks	Linalyl acetate did not mediate the cell-mediated or humoral immune response.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Gaworsky CL., Vollmuth, T.A., Dozier, M.M., Heck, J.D., Dunn, L.T., Ratajczak, H.V. and Thomas, P.T. (1994) An-Immunotoxicity Assessment of Food Flavouring Ingredients. Fd Chem. Toxic 32(5), 409415.

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)
CAS No.	125252-49-5
Method/guideline	This study was designed to investigate the Systemic toxicity of plinyl acetate and complied with the testing method described

	plinyl acetate and complied with the testing method described in Commission Directive 92/69/EEC (Method B7)
GLP	Yes
Year	1997
Species\strain	Sprague-Dawley Crl-CD Br Strain Rats
Sex	Male and Female
Route of Administration	Gavage
Doses/concentration Levels	15, 150 & 1000 mglkglday
Exposure Period	28 days
Frequency of Treatment	Daily
Control Group	Aracihs oil BP
Post Exposure Observation Period	24 hours
Remarks for Test Conditions	The test material was administered to 3 groups of 5 male and 5 female rats for 28 days. A control group of 5 male and 5 female received the vehicle only.
NOAEL (NOEL)	15 mglkglday
LOAEL (LOEL)	150 mglkglday
Toxic Response/effects by Dose Level	Increased liver and kidney wt., speckled kidney, microscopic treatment related changes in liver and kidney, accumulation of globular eosinophilic material in male kidney, centrilobular hepatocyte enlargement
Statistical Evaluation	Linear regression analysis, Followed by one way ANOVA incorporating Leven's test for homogeneity.
Remarks for Results	No deaths, no clinically observable symptoms, no effect on body weight, food consumption, hematology and clinical chemistry.
Conclusion Remarks	Oral administration of the test material to rats for a period of 28 consecutive days at the dose levels of up to 1000 mglkglday resulted in minor treatment-related changes at 1000 and 150 mglkglday. These changes were centrilobular-hepatocyte enlargement, speckled kidney and globular eosinophilic material in renal tubular epithelium.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions. Data are considered to be reliable.
Data Reliabilities Remarks	The study was performed in compliance with UK GLP and these regulations are in accordance with GLP standards published as OECD Monograph No. 45.
References	Thomas 0. N. (1997) Plinyl Acetate: Twenty-Eight day Repeated Dose Oral (Gavage) Toxicity Study in the Rat. Safepharm Laboratories, Ltd. SPL Project No. 1044/009.

Substance Name	2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol thermal rearrangement products (structurally related substance - plinyl acetate, clear colorless non-viscous liquid)

CAS No.	**125252-49-5**
Method/guideline	The study was designed to comply with the testing method described in Commission Directive 92/69/EEC (Method B7)
GLP	Yes
Year	1997
Species/strain	Sprague-Dawley Crl-CD Br Strain Rats
Sex	Male and Female
Route of Administration	Gavage
Doses/concentration Levels	0, 150, 400 & 1000 mg/kg/day
Exposure Period	28 days
Frequency of Treatment	Daily
Control Group	Arachis oil
Post Exposure Observation Period	24 hours
Remarks for Test Conditions	The study was designed to ascertain Maximum Tolerated Dose Level for 28 days study.
Actual Dose Received by Dose Level and Sex	150, 400, 1000 mglkglday
Toxic Response/effects by Dose Level	At 1000 mg/kg: Increased salivation dosing day 2, fur loss after 5 days, hunched posture due to dosing stress; At 400 or 150 mg/kg: increased salivation after Day 4 (due to impalatibility &/or local irritant nature of formulation.
Remarks for Results	No deaths, no clinically observable sings of toxicity, no effect on body wt, no macroscopic abnormalities were observed.
Conclusion Remarks	Dose levels of 1000, 100 and 15 mg/kg/day were chosen for the main study.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions. Data are considered to be reliable.
Data Reliabilities Remarks	The study was performed in compliance with UK GLP and these regulations are in accordance with GLP standards published as OECD Monograph No. 45 (OCDE/GD(92)32).
References	Thomas 0. N. (1997) (1997) Plinyl Acetate: Twenty-Eight day Repeated Dose Oral (Gavage) Toxicity Study in the Rat. Safepharm Laboratories, Ltd. SPL Project No. 1044/009.

Substance Name	Mixture of Linalool and Citronellol
CAS No.	78-70-6
Method/guideline	The test mixture was incorporated in the ration at a level designed to provide daily in the food 100 mg of the flavor blend per kg of body wt. The unsupplemented diet was fed to the controls. The rats were fed for 12 weeks.
GLP	Pre GLP
Year	1958

Species/strain	Rat (Unspecified strain)
Sex	Male and Female
Route of Administration	Feed
Doses/concentration Levels	100 mg/kg of mixture per day (50 mg/kg bw/day of linalool)
Exposure Period	12 weeks
Frequency of Treatment	Daily
Control Group	Feeding tests with a mixture of equal parts of citronellol and linalool fed at a level 100 times the estimated use level in the human diet disclosed no adverse effect on efficiency of food utilization or other observable criteria.
Remarks for Test Conditions	After 12 weeks on test, the urine of 3 rats of each sex per group was examined for the presence of sugar and albumin, blood hemoglobin levels were determined and autopsies were performed on all animals.
Toxic Response/effects by Dose Level	No adverse effects on efficiency of food utilization or other observable physiological criteria were noted.
Remarks for Results	The depression in the growth and food intake of the male rats was attributed to impalatibility of the test material at the level administered
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Food and Drug Research Laboratories (1958) Toxicological Screening of Components of Food Flavors Class VI. Citronellol and Linalool.

Substance Name	Linalyl acetate
CAS No.	115-95-7
Method/guideline	Cocarcinogenicity study
GLP	NG
Year	1971
Species/strain	Mice/ICR/Ha Swiss
Sex	Female
Route of Administration	Dermal
Doses/concentration Levels	3 mg/mouse
Exposure Period	67 weeks
Frequency of Treatment	3 times weekly
Control Group	Control groups given solvent only or untreated.
Post Exposure Observation Period	NG

Remarks for Test Conditions	The test material was applied as a solution in acetone to the backs of groups of 20 mice, 3 times per week for 67 weeks.
NOAEL (NOEL)	No carcinogenic activity at 3 mg dose
LOAEL (LOEL)	No effects at single dose level
Toxic Response/effects by Dose Level	None
Remarks for Results	Mice showing tumors for 30 days or more and greater than 1 mm in size were counted. Tumors were confirmed histologically.
Conclusion Remarks	No carcinogenic effects observed.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliabilities Remarks	Study was a cocarcinogenicity study using linalyl acetate either alone or with benzoa-pyrene as a cocarcinogen.
References	Van Duuren B., Blazej T., Goldschmidt B. Katz C., Melchionne S., and Sivak A. (1971) Cocarcinogenesis studies on mouse skin and inhibition of tumor induction. Journal of the National Cancer Institute, 45(5), 1039-1044.

Substance Name	Linalyl acetate (data on structurally related ester, linalyl isobutyrate)
CAS No.	115-95-7
Method/guideline	Method used by U.S. Food and Drug Administration.
GLP	Na
Year	1967
Species/strain	Osborne-Mendel rats
Sex	Male and Female
Route of Administration	Diet
Doses/concentration Levels	1000, 2500 or 10000 ppm
Actual Dose Received by Dose Level and Sex	NG
Exposure Period	18 weeks
Frequency of Treatment	Continuously in diet
Control Group	Yes
Post Exposure Observation Period	NG
Remarks for Test Conditions	Groups of ten male and ten female Osborne-Mendel rats were provided linalyl isobutyrate in the diet at concentrations of 0, 1000, 2500 or 10,000 ppm for 17 weeks. No vehicle was used. The diet was prepared and analyzed weekly. Measurements of body weight, food intake and general condition were recorded weekly. Hematological examinations (white cell counts, red cell counts, hemoglobins and hematocrits) were performed at the

	termination of the study. Macroscopic examination of all tissues was performed. Histopathological examination was performed on the liver, kidneys, spleen, heart, and testes of. 6-8 animals (evenly divided by sex) from the high dose and controls.
NOAEL (NOEL)	10000 ppm
LOAEL (LOEL)	No adverse effects at highest dose
Toxic Response/effects by Dose Level	None
Remarks for Results	Determination of the dietary concentration of alpha-terpinyl acetate revealed a 7% loss of test material from diet during a 7-day period. Measurements of body weight, food intake and general condition recorded weekly showed no significant differences between test and control animals at any intake level. At termination, hematological examinations revealed no difference from controls. At necropsy, no differences were reported between major organ weights of test and control. At necropsy, no differences were reported between major organ weights of test and control animals. Gross examination of tissue of all animals was unremarkable and histopathological examination revealed no treatment-related lesions.
Conclusion Remarks	This study demonstrates a NOAEL in rats of at least 10,000 ppm.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions. This study was performed by Food and Drug Administration prior to the establishment of GLP and OECD.
References	Hagan E.C., Hansen W.H., Fitzhugh O.G., Jenner P.M., Jones W.I., Taylor J.M., Long E.L., Nelson A. A., and Brouwer, J.S. (1967) Food Flavourings and Compounds of Related Structure. II, Subacute and Chronic Toxicity. Food Cosmetic Toxicology 5, 141-157.

Substance Name	Linalyl acetate (mixture of linalyl isobutyrate & geranyl acetate
CAS No.	115-95-7
Method/guideline	Method used by FDA. The test mixture was incorporated in the ration at a level designed to provide daily in the food 100 mg of the flavor blend/kg of body wt. The unsupplemented diet was fed to the controls. The rats were fed for 12 weeks.
GLP	Pre GLP
Year	1958
Species/strain	Rat (Unspecified strain)
Sex	Male and Female
Route of Administration	Feed
Doses/concentration Levels	Target dose,100 mg/kg per day of mixture. Measured dose, 112 mg/kg per day (24 mg/kg bw/day of linalyl acetate)
Exposure Period	12 weeks

Frequency of Treatment	Daily
Control Group	Male and female rats were maintained on a basal diet for 12 weeks.
Remarks for Test Conditions	After 12 wks on test, the urine of 3 rats/sex/group was examined for the presence of sugar and albumin, blood hemoglobin levels were determined and autopsies were performed on all animals.
Toxic Response/effects by Dose Level	A slight decrease in growth and efficiency of food utilization in females was concluded by the authors not to be an adverse effect.
Remarks for Results	The depression in the growth and food intake of the female rats was attributed to impalatibility of the test material at the level administered
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Trubeck Laboratories (1958) Toxicological Screening of Components of Linalyl acetate, linalyl isobutyrate, and geranyl acetate in rats. Class VIII. Unpublished Report

4.5 Reproductive Toxicity

Substance Name	Linalool (the study was conducted using natural linalool (coriander oil) 72.9% linalool)
CAS No.	78-70-6
Method/guideline	Virgin female Sprague-Dawley rats (1 O/group) were orally administered a vehicle or the test material at three dosages from one week prior to a cohabitation period through gestation, parturition and a Cday postpartum period.
Test Type	Reproductive/developmental study
GLP	NG
Year	1990
Species/Strain	Sprague-Dawley rat
Sex	Female
Route of Administration	Oral/gavage
Duration of Test	39 days
Doses/Concentration	250, 500 & 1000 mglkglday
Premating Exposure period for males	7 days
Frequency of Treatment	Daily
Control Group and Treatment	1% methylcellulose
Remarks for Test Conditions	Clinical signs, body wt & food consumption were recorded throughout the study. Mating performance, fertility, duration of

	gestation/parturition, maternal behavior, litter sized, dystocia, number of implantation sites, and gross lesions at necropsy were also examined. Offspring were examined for viability, sex, external morphology, and body wt at birth and on day 4 postpartum.
NOAEL(NOEL)	250 mglkgld (maternal NOAEL)
LOAEL(LOEL)	500 mg/kg/d (maternal)
Parental data and F1 as Appropriate	250 mglkgld: increased body weight and food consumption; 500 mg/kg/d: non-statistically significant decrease in body weight & food consumption, decreased gestation index and decreased length of gestation; 1000 mg/kg: statistically significant decrease in body weight & food consumption, statistically significant decrease in gestation index, length of gestation, and litter size
Offspring Toxicity F1 and F2	1000 mg/kg: increased number of pups dying on Days 1-4 postpartum.
Statistical Evaluation	ANOVA followed by Dunnett's test
Remarks for Results	Increased body weights were accompanied by increased food consumption. Effects were not considered adverse effects at 250 mg/kg. No effects on fertility or offspring.
Conclusion Remarks	Dose levels greater than or equal to 500 mglkgld produced toxicity in adult female rats and, at 1000 mglkgld, decreased viability of fetuses.
Data Reliabilities Qualities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The study was published in a peer-reviewed journal Teratology.
References	Vollmuth T.A., Bennett, M.B., Hoberman, A.M. and Christian, MS. (1995) An Evaluation of Food Flavoring Ingredients Using an In Vivo Reproductive and Developmental Toxicity Screening Test. Teratology 41(5): 597.

Substance Name	alpha-Terpineol acetate (The study was performed on cardamon oil, a natural mixture containing >65% tertiary terpenoid alcohol and related esters including alpha-terpineol acetate (51%) alpha terpineol, linalool, linalyl acetate, and terpinen-4-ol)
CAS No.	**80-26-2**
Method/guideline	Virgin female Sprague-Dawley rats (IO/group) were orally administered a vehicle or the test material at three dosages from one week prior to a cohabitation period through gestation, parturition and a 4 day postpartum period.
Test Type	Reproductive/developmental study
GLP	**NG**
Year	**1990**
Species/Strain	Sprague-Dawley rat
Sex	Female

Route of Administration	Oral/gavage
Duration of Test	39 days
Doses/Concentration	375, 750 & 1500 mg/kg/day
Premating Exposure period for males	7 days
Frequency of Treatment	Daily
Control Group and Treatment	1% methylcellulose
Remarks for Test Conditions	Clinical signs, body wt & food consumption were recorded throughout the study. Mating performance, fertility, duration of gestation/parturition, maternal behavior, litter sized, dystocia, number of implantation sites, and gross lesions at necropsy were also examined. Offspring were examined for viability, sex, external morphology, and body wt at birth and on day 4.
NOAEL(NOEL)	<375 mglkgld (maternal NOEAL) LOAEL at 375 mglkgld was based on decreased body weight gain and food consumption). A NOAEL for developmental toxicity in pups was 375 mg/kg/d.
LOAEL(LOEL)	375 mglkgld (maternal)
Parental data and Fl as Appropriate	375 mglkgld: non-statistically significant decrease in body weight gain and food consumption; 750 mglkgld: mortality, clinical signs, statistically significant decrease in body weight gain & food consumption, gross lesions at necropsy; 1500 mg/kg: mortality, clinical signs, statistically significant decrease in body weight gain & food consumption, gross lesions at necropsy. Small decreased in average pup weights at 750 and 1500 mg/kg/d and significant increase (P<0.01) in pup mortality at 1500 mglkgld
Offspring Toxicity F1 and F2	750 mg/kg; decreased body weights: 1500 mglkgld increased mortality and decreased body weight gain
Statistical Evaluation	ANOVA followed by Dunnett's test
Remarks for Results	Decreased body weight gain and food consumption were not statistically significant at the lowest dose.
Conclusion Remarks	Dose levels equal to 375 mglkgld resulted in depressed body weight gain and food consumption while 750 and 1500 mglkgld produced mortality and toxicity (liver weight increase and liver pathology) in adult female rats. At 750 mglkgld in offspring, decreased body weight gain during days l-4 postpartum; at 1500 mglkgld, increased mortality and decreased body weight gain of pups. The authors concluded that the test material was not uniquely toxic to the reproductive performance of female rats or the development of their offspring.
Data Reliabilities Qualities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The study was published in a peer-reviewed journal Teratology.
References	Vollmuth T.A., Bennett, M.B., Hoberman, A.M. and Christian, M.S. (1995) An Evaluation of Food Flavoring Ingredients Using an In Vivo Reproductive and Developmental Toxicity Screening Test. Teratology 41(5): 597.

4.6 Developmental/Teratogenicity Toxicity

Substance Name	Pine oil blend (blend compose of five commercial pine oil samples. Range of composition was 35- *76.7% alpha-* and gamma-terpineol, l-l 3.1% other terpineol isomers, O-14.6% secondary terpene alcohols, O.l-10% terpene hydrocarbons)
CAS No.	8002-09-3
Method/guideline	The test substance was administered on days 6 through 20 of gestation to pregnant rats at the dosage of 0, 50, 100, 500, 750, or 1000 mglkglday at a volume of 10 ml/kg. On day 20 of presumed gestation, all rats were terminated by asphyxiation with C02.
Test Type	Dose range finding study of Teratology study
GLP	Yes
Year	1988
Species/strain	Crl:CD(SD)BR pregnant rats
Sex	Female
Route of Administration	Gavage
Duration of Test	14 days
Doses/concentration Levels	0, 100, 500, 750 or 1000 mglkglday
Exposure Period	14 days
Control Group and Treatment	Corn oil
Remarks for Test Conditions	Laparotomies were performed, corpora lutea were counted, and the uterus of each rat was removed, weighed and then examined for number, placement and viability of implantations. Live fetuses were weighed, sexed and gross external alternations were identified. Soft tissue and skeletal evaluations were not performed for this dosage-range (pilot study.)
Maternal Data with Dose Level	There were no deaths or abortions during the course of this study. Necropsy revealed no gross lesions. Excess salivation occurred within 30 min at dosage 100 and above, local alopecia, inhibition of average maternal body weight, decrease in feed consumption for 3 highest doses. At 750 & 1000 mg/kg, reduced average gravid uterine weight,
Fetal Data with Dose Level	Decreased fetal body weight in dosages 100 mg/kg and above. At 500 & 750 mg/kg, slight increase in average number of resorptions/litter.
Remarks for Results	On the basis of this study, dosages of 0, 50, 600 and 1200 mg/kg/day of Pine oil blend were recommended for definitive developmental toxicity study.
Conclusion Remarks	On the basis of this study, dosages of 0, 50, 600 and 1200 mg/kg/day of Pine oil blend were recommended for definitive developmental toxicity study.

Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliabilities Remarks	The study was conducted in accordance with GLP guidelines
References	Dearlove G. E. (1987) Dosage-Range Developmental Toxicity Study of Pine Oil Blend 1687 Administered Orally Via Gavage to Crl:CD(SD)BR Presumed Pregnant Rats (Pilot Study). Appendix IV to Parent, R.A. (1988). Teratogenicity Study in Albino Rats with Pine Oil Blend. A Report Submitted by Pine Oil Joint Venture to Chemical Specialties Manufacturers Association,

Substance Name	Pine oil blend (blend compose of five commercial pine oil samples. Range of composition was 35- 76.7% alpha- and gamma-terpineol, l-l 3.1% other terpineol isomers, 0-14.6% secondary terpene alcohols, 0.1-10% terpene hydrocarbons)
CAS No.	8002-09-3
Method/guideline	Pine oil Blend was administered by gavage at the doses of 0, 50, 600 or 1200 mglkglday to pregnant rats on gestation days 6 through 20. On day 20 of presumed gestation, rats were sacrificed.
Test **Type**	Teratology study
GLP	Yes
Year	1988
Species/strain	Crl:CD(SD)BR pregnant rats
Sex	Female
Route of Administration	Gavage
Duration of Test	14 days (Gestation day 6 through 20)
Doses/concentration Levels	0, 50, 600 or 1200 mglkglday
Exposure Period	14 days
Frequency of Treatment	Daily
Control Group and Treatment	Corn oil
Remarks for Test Conditions	The rats were examined for pregnancy, number and placement of implantations, early and late resorptions, live and dead fetuses, and number of corpora lutea. Fetuses were subsequently weighed and evaluated for both soft and hard tissue abnormalities.
NOAEL Maternal Toxicity	>50 mg/kg
LOAEL Maternal Toxicity	<600 mg/kg
Maternal Data with Dose Level	At 600 & 1200 mglkglday: maternal toxicity, decreased food consumption, body weight gains, excess salivation, alopecia, ungroomed coat, ataxia, decreased motor activity, impaired righting reflex and urine stained abdominal fur. Six of the 25

	rats in 1200 mg/kg died and necropsies revealed that adrenal weights were significantly increased in these rats.
Fetal Data with Dose Level	Increased incidences of delayed fetal ossification, delayed brain development, decreased fetal weights, increased embryofetal mortality, and sunken eyes bulge with associated soft and hard tissue findings at 1200 mg/kg, a dosage that also resulted in maternal death and a low incidence of embryo-fetal death (resorption).
Statistical Evaluation	Bartlett, Kruskall-Walks, Dunn's test, Dunnett's
Conclusion Remarks	Pine oil blend is not expected to produce adverse effects on embryofetal development except at doses that are also maternally toxic. The maternal and developmental NOEL for Pine Oil under the conditions of this study was greater than 50 mglkglday but less than 600 mglkglday.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions
Data Reliabilities Remarks	The study was conducted in accordance to GLP guidelines.
References	Parent R.A. (1988) Teratogenicity Study in Albino Rats with Pine Oil Blend. A Report Submitted by Pine Oil Joint Venture to Chemical Specialties Manufacturers Association.