201-16410B

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IUCLID

Data Set

Existing Chemical	:	ID: 116265-68-0
Producer related part		
Company	:	Epona Associates, LLC
Creation date	:	09.11.2006
Substance related part		
Company	:	Epona Associates, LLC
Creation date	:	09.11.2006
Status	:	
Memo	:	Chemtura
Printing date	:	09.11.2006
Revision date	:	
Date of last update	:	09.11.2006
Number of pages	:	29
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1. General Information

Id 116265-68-0
Date 09.11.2006

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name	:	Phosphorous acid, triphenyl ester, reaction products with dipropylene glycol
Smiles Code	:	
Molecular formula	:	
Molecular weight	:	
Petrol class	:	
Remark	:	D 25 207 = 60-100% poly (dipropyleneglycol) phenyl phosphite (CAS 80584-86-7), 5-10% triphenyl phosphite and 0.1-1% phenol. Phosphorous acid tri phenyl ester reaction products with dipropylene glycol (CAS No. 116265-68-0) is intended to cover all the potential products derived from the reaction which would include: commercial products Weston DHOP (D 25 207) and THOP (which include CAS No. 80584-86-7 Poly (dipropyleneglycol) phenyl phosphate) and Weston PTP (which includes CAS No. 13474-96-9 Heptakis (dipropyleneglycol) triphosphite. Data from these potential products are relevant for the sponsored substance. Weston (R) THOP = >30-<60% tetraphenyl dipropylene glycol diphosphate (CAS 80584-86-7) and >15-<40 triphenyl phosphite (CAS 101-02-0).

09.11.2006

1.1.1 GENERAL SUBSTANCE INFORMATION

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Sublimation :
Method :
Year : 2006
GLP : no data
Test substance : other TS

Remark : Substance is a liquid. Melting point not applicable.
Test substance : Weston THOP (which include CAS No. 80584-86-7 Poly (dipropyleneglycol) phenyl phosphate)
Reliability : (2) valid with restrictions
09.11.2006 (2)

Sublimation :
Method :
Year : 2006
GLP : no data
Test substance : other TS

Remark : Substance is a liquid. Melting point not applicable.
Test substance : Weston DHOP (which include CAS No. 80584-86-7 Poly (dipropyleneglycol) phenyl phosphate)
Reliability : (2) valid with restrictions
Internal company data
09.11.2006 (1)

Sublimation :
Method :
Year : 2006
GLP : no data
Test substance : other TS

Remark : Substance is a liquid. Melting point not applicable.
Test substance : Weston PTP (which includes CAS No. 13474-96-9 Heptakis (dipropyleneglycol) triphosphite.
Reliability : (2) valid with restrictions
Internal company data
09.11.2006 (3)

2.2 BOILING POINT

Value : 942 °C at 1013 hPa
Decomposition :
Method : other: calculated
Year : 2006
GLP : no
Test substance : other TS

Method :

MPBPWIN (v1.41) Program
==========
Experimental Database Structure Match: no data

SMILES :
CC(OP(OC(COCC(C)O)C)OC(C)COCC(C)OP(OC(C)COCC(C)O)OC(C)C
OCC(C)O)COCC(O

P(OC(C)COCC(O)C)OC(COCC(C)O)C)C
CHEM : Phosphorous acid, 2-(2-hydroxypropoxy)-1-methylethyl bis[13-hydroxy-7
-[2-(2-hydroxypropoxy)-1-methylethoxy]-1,5,9-trimet
MOL FOR: C42 H89 O21 P3
MOL WT : 1023.09

Result :

MPBPWIN (v1.41) Program Results:
==========
Experimental Database Structure Match: no data

SUMMARY MPBPWIN v1.41 ----------

Boiling Point: 942.82 deg C (Adapted Stein and Brown Method)

Melting Point: 349.84 deg C (Adapted Joback Method)
Melting Point: 349.84 deg C (Gold and Ogle Method)
Mean Melt Pt : 349.84 deg C (Joback; Gold,Ogle Methods)
Selected MP: 349.84 deg C (Weighted Value)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	14	-CH3	21.98	307.72
Group	14	-CH2-	24.22	339.08
Group	14	>CH-	11.86	166.04
Group	16	-O- (nonring)	25.16	402.56
Group	3	>P-	43.75	131.25
Group	5	-OH (secondary)	80.63	403.15
*		Equation Constant		198.18

RESULT-uncorr| BOILING POINT in deg Kelvin | 1947.98
RESULT- corr | BOILING POINT in deg Kelvin | 1215.98
| BOILING POINT in deg C | 942.82

Test substance : CAS No. 13474-96-9 Heptakis (dipropyleneglycol) triphosphite.
Reliability : (2) valid with restrictions
Data derived from an estimation program

09.11.2006 (4)

Value : 1866 °C at 1013 hPa
Decomposition :
Method :
Year : 2006
GLP : no
Test substance : other TS

Method : MPBPWIN (v1.41) Program Results:
==========
Experimental Database Structure Match: no data

SMILES :
CC(OP(Oc2ccccc2)Oc3ccccc3)COCC(C)OP(Oc4ccccc4)OC(C)COCC(C)OP(Oc5ccccc

5)OC(C)COCC(C)OP(Oc6ccccc6)OC(C)COCC(C)OP(OC(C)COCC(C)OP(Oc7ccccc7)OC

(COCC(C)OP(Oc8ccccc8)OC(C)COCC(OP(Oc9ccccc9)Oc0ccccc0)C)C)O
c1ccccc1
CHEM : Phosphorous acid, oxybis(1-methyl-2,1-ethanediyl) P,P -
bis(1,5,9,13,1
7,21-hexamethyl-7,15,23,23-tetraphenoxy-3,6,8,11,14
MOL FOR: C102 H134 O31 P8
MOL WT : 2103.98

Result : SUMMARY MPBPWIN v1.41 ----------

Boiling Point: 1866.09 deg C (Adapted Stein and Brown Method)

Melting Point: 349.84 deg C (Adapted Joback Method)
Melting Point: 349.84 deg C (Gold and Ogle Method)
Mean Melt Pt : 349.84 deg C (Joback; Gold,Ogle Methods)
Selected MP: 349.84 deg C (Weighted Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 1866.09 deg C (estimated))
(Using MP: 349.84 deg C (estimated))
VP: 0 mm Hg (Antoine Method)
VP: 3E-051 mm Hg (Modified Grain Method)
VP: 4.03E-051 mm Hg (Mackay Method)
Selected VP: 0 mm Hg (Modified Grain Method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	14	-CH3	21.98	307.72
Group	14	-CH2-	24.22	339.08
Group	14	>CH-	11.86	166.04
Group	31	-O- (nonring)	25.16	779.96
Group	8	>P-	43.75	350.00
Group	50	CH (aromatic)	28.53	1426.50
Group	10	-C (aromatic)	30.76	307.60
*		Equation Constant		198.18

RESULT-uncorr| BOILING POINT in deg Kelvin | 3875.08
RESULT- corr | BOILING POINT in deg Kelvin | 2139.25
| BOILING POINT in deg C | 1866.09

Test substance : CAS No. 80584-86-7 Poly (dipropyleneglycol) phenyl phosphate)
Reliability : (2) valid with restrictions
Data derived from an estimation program

09.11.2006 (4)

2.3 DENSITY

Type : density
Value : .9 g/cm³ at 25 °C
Method :
Year : 2006
GLP : no data
Test substance : other TS

Test substance : Weston PTP (which includes CAS No. 13474-96-9 Heptakis (dipropyleneglycol) triphosphite.
Reliability : (2) valid with restrictions
Internal company data

09.11.2006 (3)

Type : density
Value : 1.1 g/cm³ at 25 °C
Method :
Year : 2006
GLP : no data
Test substance : other TS

Test substance : Weston THOP (which include CAS No. 80584-86-7 Poly (dipropyleneglycol) phenyl phosphate)
Reliability : (2) valid with restrictions
Internal company data

09.11.2006 (2)

Type : density
Value : 1.18 g/cm³ at 25 °C
Method :
Year : 2006
GLP : no data
Test substance : other TS

Test substance : Weston DHOP (which include CAS No. 80584-86-7 Poly (dipropyleneglycol) phenyl phosphate)
Reliability : (2) valid with restrictions
Internal company data

09.11.2006 (1)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Decomposition :
Method : other (calculated)
Year : 2006
GLP : no
Test substance : other TS

Method : MPBPWIN (v1.41) Program
==========
Experimental Database Structure Match: no data

SMILES :
CC(OP(OC(COCC(C)O)C)OC(C)COCC(C)OP(OC(C)COCC(C)O)OC(C)C
OCC(C)O)COCC(O
P(OC(C)COCC(O)C)OC(COCC(C)O)C)C
CHEM : Phosphorous acid, 2-(2-hydroxypropoxy)-1-methylethyl bis[13-hydroxy-7
-[2-(2-hydroxypropoxy)-1-methylethoxy]-1,5,9-trimet
MOL FOR: C42 H89 O21 P3
MOL WT : 1023.09

Result : MPBPWIN (v1.41) Program Results:
==========
Experimental Database Structure Match: no data

---------- SUMMARY MPBPWIN v1.41

Vapor Pressure Estimations (25 deg C):
(Using BP: 942.82 deg C (estimated))
(Using MP: 349.84 deg C (estimated))
VP: 8.79E-065 mm Hg (Antoine Method)
VP: 1.27E-030 mm Hg (Modified Grain Method)
VP: 3.76E-023 mm Hg (Mackay Method)
Selected VP: 1.27E-030 mm Hg (Modified Grain Method)

Test substance : CAS No. 13474-96-9 Heptakis (dipropyleneglycol) triphosphite.
Reliability : (2) valid with restrictions
Data derived from an estimation program

09.11.2006 (4)

Decomposition :
Method : other (calculated)
Year : 2006
GLP : no
Test substance : other TS

Method : MPBPWIN (v1.41) Program
==========
Experimental Database Structure Match: no data

SMILES :
CC(OP(Oc2ccccc2)Oc3ccccc3)COCC(C)OP(Oc4ccccc4)OC(C)COCC(C)O
P(Oc5ccccc

5)OC(C)COCC(C)OP(Oc6ccccc6)OC(C)COCC(C)OP(OC(C)COCC(C)OP(
Oc7ccccc7)OC

(COCC(C)OP(Oc8ccccc8)OC(C)COCC(OP(Oc9ccccc9)Oc0ccccc0)C)C)O
c1ccccc1
CHEM : Phosphorous acid, oxybis(1-methyl-2,1-ethanediyl) P,P -
bis(1,5,9,13,1
7,21-hexamethyl-7,15,23,23-tetraphenoxy-3,6,8,11,14
MOL FOR: C102 H134 O31 P8
MOL WT : 2103.98
-

Result : MPBPWIN (v1.41) Program Results:
==========
Experimental Database Structure Match: no data

- SUMMARY MPBPWIN v1.41 ----------

Vapor Pressure Estimations (25 deg C):
(Using BP: 1866.09 deg C (estimated))
(Using MP: 349.84 deg C (estimated))
VP: 0 mm Hg (Antoine Method)
VP: 3E-051 mm Hg (Modified Grain Method)
VP: 4.03E-051 mm Hg (Mackay Method)
Selected VP: 0 mm Hg (Modified Grain Method)

Test substance : CAS No. 80584-86-7 Poly (dipropyleneglycol) phenyl phosphate)
Reliability : (2) valid with restrictions
Data derived from an estimation program

09.11.2006 (4)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water

Log pow : -3.41 at 25 °C
pH value :
Method : other (calculated)
Year : 2006
GLP : no
Test substance : other TS

Method : KOWWIN Program (v1.67) :
==========

SMILES :
CC(OP(OC(COCC(C)O)C)OC(C)COCC(C)OP(OC(C)COCC(C)O)OC(C)C
OCC(C)O)COCC(O
P(OC(C)COCC(O)C)OC(COCC(C)O)C)C
CHEM : Phosphorous acid, 2-(2-hydroxypropoxy)-1-methylethyl bis[13-
hydroxy-7
-[2-(2-hydroxypropoxy)-1-methylethoxy]-1,5,9-trimet
MOL FOR: C42 H89 O21 P3
MOL WT : 1023.09

Result : KOWWIN Program (v1.67) Results:
==========

Log Kow(version 1.67 estimate): -3.41

```
TYPE | NUM | LOGKOW FRAGMENT DESCRIPTION|COEFF |VALUE
-------+-----+-------------------------------------------+
Frag |14 | -CH3 [aliphatic carbon]  | 0.5473| 7.6622
Frag |14| -CH2-[aliphatic carbon]    | 0.4911| 6.8754
Frag |14| -CH [aliphatic carbon]  | 0.3614|  5.0596
Frag| 5 | -OH[hydroxy, aliphatic attach]|-1.4086| -7.0430
Frag |7| -O-[oxygen, aliphatic attach] |-1.2566| -8.7962
Frag| 3| >P- [phosphine type] |-0.5000 | -1.5000
Frag|9| -O-P[phosphine phosphorus attach] |-0.7000  | -6.3000
 Factor|  1  | Multi-alcohol correction |0.4064 | 0.4064
 Const |     |  Equation Constant     |         | 0.2290
-------+-----+-------------------------------------------+---------+--------
                                          Log Kow  =  -3.4066
```

Test substance : CAS No. 13474-96-9 Heptakis (dipropyleneglycol) triphosphite.
Data derived from an estimation program

09.11.2006 (4)

Partition coefficient : octanol-water
Log pow : 20.215 at °C
pH value :
Method : other (calculated)
Year : 2006
GLP : no
Test substance : other TS

Method : Log Kow(version 1.67):

SMILES :
CC(OP(Oc2ccccc2)Oc3ccccc3)COCC(C)OP(Oc4ccccc4)OC(C)COCC(C)O
P(Oc5ccccc

5)OC(C)COCC(C)OP(Oc6ccccc6)OC(C)COCC(C)OP(OC(C)COCC(C)OP(
Oc7ccccc7)OC

(COCC(C)OP(Oc8ccccc8)OC(C)COCC(OP(Oc9ccccc9)Oc0ccccc0)C)C)O
c1ccccc1
CHEM : Phosphorous acid, oxybis(1-methyl-2,1-ethanediyl) P,P -

bis(1,5,9,13,1
7,21-hexamethyl-7,15,23,23-tetraphenoxy-3,6,8,11,14
MOL FOR: C102 H134 O31 P8
MOL WT : 2103.98

Result :

```
TYPE  |NUM| LOGKOW FRAGMENT DESCRIPTION|COEFF| VALUE
-------+-----+-----------------------------------------+
Frag |14  | -CH3[aliphatic carbon]     |0.5473| 7.6622
Frag |14  |-CH2- [aliphatic carbon]    |0.4911|6.8754
Frag|14 |  -CH  [aliphatic carbon]    |0.3614 |5.0596
Frag|7  |  -O-  [oxygen, aliphatic attach]|-1.2566|-8.7962
Frag| 60| Aromatic Carbon            |0.2940 |17.6400
Frag|10 | -O-P  [aromatic attach]   |0.5345 | 5.3450
Frag| 8 |  >P-  [phosphine type]    |-0.5000  | -4.0000
Frag| 14|-O-P[phosphine phosphorus attach]|-0.7000|-9.8000
Const|    |  Equation Constant     |        |  0.2290
-------+-----+-----------------------------------------+
                                        Log Kow  =  20.2150
```

Test substance : CAS No. 80584-86-7 Poly (dipropyleneglycol) phenyl phosphate)
Reliability : (2) valid with restrictions
Data derived from an estimation program

09.11.2006 (4)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : at °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description : not soluble
Stable :
Deg. product :
Method :
Year : 2006
GLP : no data
Test substance : other TS

Test substance : Weston THOP (which include CAS No. 80584-86-7 Poly (dipropyleneglycol) phenyl phosphate)
Reliability : (2) valid with restrictions
Internal company data

09.11.2006 (2)

Solubility in : Water
Value : at °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description : not soluble
Stable :
Deg. product :
Method :
Year : 2006
GLP : no data
Test substance : other TS

Remark : Insoluble, slowly hydrolyzes
Test substance : Weston PTP (which includes CAS No. 13474-96-9 Heptakis (dipropyleneglycol) triphosphite.
Reliability : (2) valid with restrictions
Internal company data

09.11.2006 (3)

Solubility in : Water
Value : at °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description : not soluble
Stable :
Deg. product :
Method : other: calculated
Year : 2006
GLP : no
Test substance : other TS

Method : SMILES :
CC(OP(Oc2ccccc2)Oc3ccccc3)COCC(C)OP(Oc4ccccc4)OC(C)COCC(C)OP(Oc5ccccc

5)OC(C)COCC(C)OP(Oc6ccccc6)OC(C)COCC(C)OP(OC(C)COCC(C)OP(Oc7ccccc7)OC

(COCC(C)OP(Oc8ccccc8)OC(C)COCC(OP(Oc9ccccc9)Oc0ccccc0)C)C)Oc1ccccc1
CHEM : Phosphorous acid, oxybis(1-methyl-2,1-ethanediyl) P,P - bis(1,5,9,13,1
7,21-hexamethyl-7,15,23,23-tetraphenoxy-3,6,8,11,14
MOL FOR: C102 H134 O31 P8
MOL WT : 2103.98
Result : Water Sol from Kow (WSKOW v1.41) Results:
==========

Water Sol: 3.455e-026 mg/L
WSKOW v1.41 Results ----------
Log Kow (estimated) : 20.22
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: 20.22

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
(used when Melting Point NOT available)

Correction(s): Value
--- ---
No Applicable Correction Factors

Log Water Solubility (in moles/L) : -31.785
Water Solubility at 25 deg C (mg/L): 3.455e-026
Test substance : CAS No. 80584-86-7 Poly (dipropyleneglycol) phenyl phosphate)
Reliability : (2) valid with restrictions
Data derived from an estimation program

09.11.2006 (4)

Solubility in : Water

Value	:	185 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	2006
GLP	:	no
Test substance	:	other TS

Method : Water Sol from Kow (WSKOW v1.41)
==========

SMILES :
CC(OP(OC(COCC(C)O)C)OC(C)COCC(C)OP(OC(C)COCC(C)O)OC(C)C
OCC(C)O)COCC(O
P(OC(C)COCC(O)C)OC(COCC(C)O)C)C
CHEM : Phosphorous acid, 2-(2-hydroxypropoxy)-1-methylethyl bis[13-hydroxy-7
-[2-(2-hydroxypropoxy)-1-methylethoxy]-1,5,9-trimet
MOL FOR: C42 H89 O21 P3
MOL WT : 1023.09
---------- WSKOW v1.41 Results ----------
Log Kow (estimated) : -3.41
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: -3.41

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
(used when Melting Point NOT available)

Correction(s): Value
---------- -----
No Applicable Correction Factors

Log Water Solubility (in moles/L) : -3.743
Water Solubility at 25 deg C (mg/L): 185

Result : Water Sol from Kow (WSKOW v1.41) Results:
==========

Water Sol: 185 mg/L

SMILES :
CC(OP(OC(COCC(C)O)C)OC(C)COCC(C)OP(OC(C)COCC(C)O)OC(C)C
OCC(C)O)COCC(O
P(OC(C)COCC(O)C)OC(COCC(C)O)C)C
CHEM : Phosphorous acid, 2-(2-hydroxypropoxy)-1-methylethyl bis[13-hydroxy-7
-[2-(2-hydroxypropoxy)-1-methylethoxy]-1,5,9-trimet
MOL FOR: C42 H89 O21 P3
MOL WT : 1023.09
---------- WSKOW v1.41 Results ----------
Log Kow (estimated) : -3.41
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: -3.41

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
(used when Melting Point NOT available)

Correction(s):	Value
No Applicable Correction Factors	

Log Water Solubility (in moles/L) : -3.743
Water Solubility at 25 deg C (mg/L): 185

Test substance : CAS No. 13474-96-9 Heptakis (dipropyleneglycol) triphosphite.
Reliability : (2) valid with restrictions
Data derived from an estimation program

09.11.2006 (4)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type : air
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer :
Rate constant : .000000000583 cm³/(molecule*sec)
Degradation : 50 % after 0 day(s)
Deg. product :
Method : other (calculated)
Year : 2006
GLP : no
Test substance : other TS

Method : AOP Program (v1.91)
==========
SMILES :
CC(OP(OC(COCC(C)O)C)OC(C)COCC(C)OP(OC(C)COCC(C)O)OC(C)C
OCC(C)O)COCC(O
P(OC(C)COCC(O)C)OC(COCC(C)O)C)C
CHEM : Phosphorous acid, 2-(2-hydroxypropoxy)-1-methylethyl bis[13-hydroxy-7
-[2-(2-hydroxypropoxy)-1-methylethoxy]-1,5,9-trimet
MOL FOR: C42 H89 O21 P3
MOL WT : 1023.09

Result : AOP Program (v1.91) Results:
==========
SUMMARY (AOP v1.91): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 582.4637 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.7000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 583.1637 E-12 cm3/molecule-sec
HALF-LIFE = 0.018 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 13.206 Min
---------- SUMMARY (AOP v1.91): OZONE REACTION ----------

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches

Test substance : CAS No. 13474-96-9 Heptakis (dipropyleneglycol) triphosphite.
Reliability : (2) valid with restrictions
Data derived from an estimation program

09.11.2006 (4)

Type : air
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer :

Conc. of sensitizer :
Rate constant : .000000000541 cm³/(molecule*sec)
Degradation : 50 % after 0 day(s)
Deg. product :
Method :
Year : 2006
GLP : no
Test substance : other TS

Method : AOP Program (v1.91)
SMILES :
CC(OP(Oc2ccccc2)Oc3ccccc3)COCC(C)OP(Oc4ccccc4)OC(C)COCC(C)O
P(Oc5ccccc

5)OC(C)COCC(C)OP(Oc6ccccc6)OC(C)COCC(C)OP(OC(C)COCC(C)OP(
Oc7ccccc7)OC

(COCC(C)OP(Oc8ccccc8)OC(C)COCC(OP(Oc9ccccc9)Oc0ccccc0)C)C)O
c1ccccc1
CHEM : Phosphorous acid, oxybis(1-methyl-2,1-ethanediyl) P,P -
bis(1,5,9,13,1
7,21-hexamethyl-7,15,23,23-tetraphenoxy-3,6,8,11,14
MOL FOR: C102 H134 O31 P8
MOL WT : 2103.98

Result : AOP Program (v1.91) Results:
==========
SUMMARY (AOP v1.91): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 504.9969 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings = 36.1410 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 541.1379 E-12 cm3/molecule-sec
HALF-LIFE = 0.020 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 14.231 Min
..... ** Designates Estimation(s) Using ASSUMED Value(s)
---------- SUMMARY (AOP v1.91): OZONE REACTION ----------

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches

Test substance : CAS No. 80584-86-7 Poly (dipropyleneglycol) phenyl phosphate)
Reliability : (2) valid with restrictions
Data derived from an estimation program

09.11.2006 (4)

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media :
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: calculated
Year : 2006

Method : Level III Fugacity Model (Full-Output):
==========
Chem Name : Phosphorous acid, oxybis(1-methyl-2,1-ethanediyl) P,P - bis(1,5,9
13,17,21-hexamethyl-7,15,23,23-tetraphenoxy-3,6,8,11,14
Molecular Wt: 2104
Henry's LC : 8.01e+010 atm-m3/mole (calc VP/Wsol)
Vapor Press : 1e-015 mm Hg (Zero default)
Liquid VP : 1.63e-012 mm Hg (super-cooled)
Melting Pt : 350 deg C (Mpbpwin program)
Log Kow : 20.2 (Kowwin program)
Soil Koc : 6.8e+019 (calc by model)

Result : Level III Fugacity Model (Full-Output):
==========

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.00404	0.474	1000
Water	1.27	3.6e+003	1000
Soil	32	3.6e+003	1000
Sediment	66.8	1.44e+004	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.4e-019	974	6.67	32.5	0.222
Water	3.63e-010	40.5	210	1.35	7.01
Soil	6.84e-012	1.02e+003	0	33.9	0
Sediment	6.43e-010	531	221	17.7	7.36

Persistence Time: 5.51e+003 hr
Reaction Time: 6.45e+003 hr
Advection Time: 3.78e+004 hr
Percent Reacted: 85.4
Percent Advected: 14.6

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 0.4745
Water: 3600
Soil: 3600
Sediment: 1.44e+004
Biowin estimate: -1.291 (recalcitrant)

Advection Times (hr):
Air: 100
Water: 1000

Sediment: 5e+004

Test substance : CAS No. 80584-86-7 Poly (dipropyleneglycol) phenyl phosphate)
Reliability : (2) valid with restrictions
Data derived from an estimation program

09.11.2006 (4)

Type : fugacity model level III
Media :
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: calculated
Year : 2006

Method : Level III Fugacity Model (Full-Output):
==========
Chem Name : Phosphorous acid, 2-(2-hydroxypropoxy)-1-methylethyl bis[13-hydr
xy-7-[2-(2-hydroxypropoxy)-1-methylethoxy]-1,5,9-trimet
Molecular Wt: 1023.1
Henry's LC : 1.25e-033 atm-m3/mole (Henrywin program)
Vapor Press : 1.27e-030 mm Hg (Mpbpwin program)
Liquid VP : 2.07e-027 mm Hg (super-cooled)
Melting Pt : 350 deg C (Mpbpwin program)
Log Kow : -3.41 (Kowwin program)
Soil Koc : 0.00016 (calc by model)

Result : Level III Fugacity Model (Full-Output):
==========

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	5.45e-006	0.44	1000
Water	54.4	3.6e+003	1000
Soil	45.5	3.6e+003	1000
Sediment	0.106	1.44e+004	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.22e-037	0.35	0.00222	0.0117	7.4e-005
Water	1.35e-038	427	2.22e+003	14.2	73.9
Soil	4.19e-037	356	0	11.9	0
Sediment	1.32e-038	0.208	0.0863	0.00692	0.00288

Persistence Time: 1.36e+003 hr
Reaction Time: 5.2e+003 hr
Advection Time: 1.84e+003 hr
Percent Reacted: 26.1
Percent Advected: 73.9

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 0.4402
Water: 3600
Soil: 3600
Sediment: 1.44e+004
Biowin estimate: 1.677 (recalcitrant)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Test substance : CAS No. 13474-96-9 Heptakis (dipropyleneglycol) triphosphite.
Reliability : (2) valid with restrictions
Data derived from an estimation program

09.11.2006 (4)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	> 5000 mg/kg bw
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	
Year	:	2006
GLP	:	no data
Test substance	:	other TS
Result	:	estimate
Test substance	:	Weston THOP (which include CAS No. 80584-86-7 Poly (dipropyleneglycol) phenyl phosphate)
Reliability	:	(2) valid with restrictions Internal company data

09.11.2006 (2)

Type	:	LD50
Value	:	> 2000 mg/kg bw
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	
Year	:	2006
GLP	:	no data
Test substance	:	other TS
Test substance	:	Weston DHOP (which include CAS No. 80584-86-7 Poly (dipropyleneglycol) phenyl phosphate)
Reliability	:	(2) valid with restrictions Internal company data

09.11.2006 (1)

Type	:	LD50
Value	:	> 10000 mg/kg bw
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	
Year	:	2006
GLP	:	no data
Test substance	:	other TS
Test substance	:	Weston PTP (which includes CAS No. 13474-96-9 Heptakis

(dipropyleneglycol) triphosphite.

Reliability : (2) valid with restrictions
Internal company data

09.11.2006 (3)

5.1.2 ACUTE INHALATION TOXICITY

Type : LC50
Value : > 2 mg/l
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Exposure time :
Method :
Year : 2006
GLP : no data
Test substance : other TS

Test substance : Weston DHOP (which include CAS No. 80584-86-7 Poly (dipropyleneglycol) phenyl phosphate)

Reliability : (2) valid with restrictions
Internal company data

09.11.2006 (1)

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50
Value : > 2000 mg/kg bw
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method :
Year : 2006
GLP : no data
Test substance : other TS

Test substance : Weston THOP (which include CAS No. 80584-86-7 Poly (dipropyleneglycol) phenyl phosphate)

Reliability : (2) valid with restrictions
Internal company data

09.11.2006 (2)

Type : LD50
Value : > 200 mg/kg bw
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method :
Year : 2006

GLP	:	no data
Test substance	:	other TS
Test substance	:	Weston DHOP (which include CAS No. 80584-86-7 Poly (dipropyleneglycol) phenyl phosphate)
Reliability	:	(2) valid with restrictions Internal company data

09.11.2006 (1)

Type	:	LD50
Value	:	> 200 - mg/kg bw
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	
Year	:	2006
GLP	:	no data
Test substance	:	other TS
Test substance	:	Weston PTP (which includes CAS No. 13474-96-9 Heptakis (dipropyleneglycol) triphosphite.
Reliability	:	(2) valid with restrictions Internal company data

09.11.2006 (3)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
Vehicle	:	
PDII	:	
Result	:	
Classification	:	
Method	:	
Year	:	2006
GLP	:	no data
Test substance	:	other TS
Result	:	contact with the skin did not produce ulceration or necrosis
Test substance	:	Weston DHOP (which include CAS No. 80584-86-7 Poly (dipropyleneglycol) phenyl phosphate)
Reliability	:	(2) valid with restrictions Internal company data

09.11.2006 (1)

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

9. References

(1) Chemtura (2006) MSDS D 25-207. 01/08/2006

(2) Chemtura (2006) MSDS Weston (R) THOP. 01/08/2006

(3) Chemtura (2006) Weston (R) PTP. 01/05/2006

(4) EpiWin (v. 3.11)

10. Summary and Evaluation

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT