Completed Sustainable Futures

Summary Assessment

Using

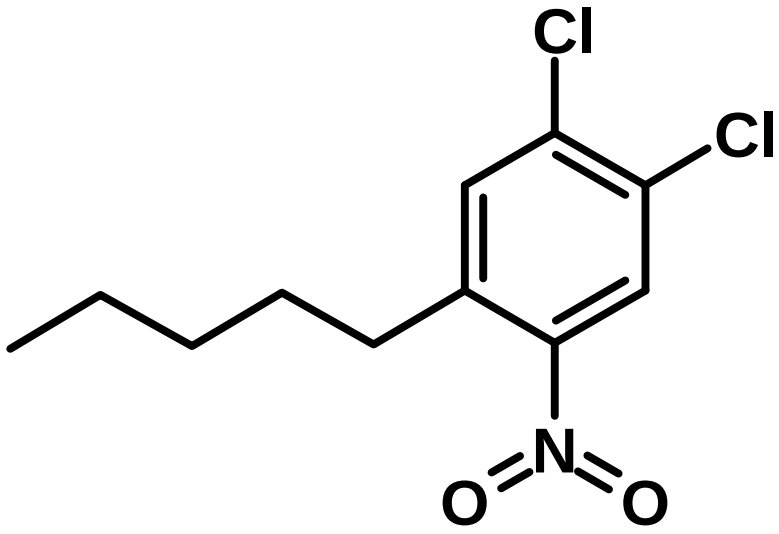
P2 Framework Models

This document was developed to help compile estimation results from U.S. EPA OPPT's P2 Framework Models and is used by OPPT during Sustainable Futures (SF) training described at www.epa.gov/oppt/sf. Participants in the voluntary SF Pilot Project are asked to submit the information contained in this assessment along with their SF PMNs in their choice of format. **Use of this specific format is not mandatory.**

Chemical Assessed (Sample Chemical 1):
1,2-Dichloro-4-nitro-5-pentylbenzene

CAS Registry Number:
Not Located

Participant Name:
SF Trainers

Record ID: Training Session Sample Chemical 1	CAS No.
	**MW**: 262.14
	MF: $C_{11}H_{13}Cl_2N_1O_2$
	Physical Form: Solid
	Submitter: SF Trainers, Inc.
	Trade Name: INTERSYN
	Use: Synthetic Intermediate
	Production Volume: 50,000 kg/yr

SMILES: c1(cc(c(cc1Cl)CCCCC)(N(=O)=O))Cl

Name: 1,2-dichloro-4-nitro-5-pentylbenzene

Synonyms: Pentyl, dichloro, nitrobenzene

SUSTAINABLE FUTURES SUMMARY:

Concern Level	HIGH	MODERATE	LOW
Persistence	X		
Bioconcentration		X	
Cancer Health Hazard		X	
Non-Cancer Health Hazard		X	
Aquatic Toxicity Hazard	X		
Is the chemical predicted to be a PBT by PBT Profiler?	YES		
Overall Hazard Concern	Human Health Hazard: High Aquatic Hazard: High		
Overall Risk	Human Health Risk: Potential risk exists Aquatic Risk: Potential risk exists		

CAS No.	Submitter: SF Trainers, Inc.
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	114 (EPI)
Boiling Point (deg C)	337 (EPI)
Boiling Point Pressure (mm Hg)	760 (EPI)
Vapor Pressure (mm Hg)	3.4×10^{-5} (EPI)
Water Solubility	0.13 mg/L (EPI)
Octanol/Water Partition Coefficient - Log K_{ow}	5.61 (EPI)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC	1.5×10^{-4} atm/m^3-mole (EPI)
Soil Adsorption Coefficient – Log K_{oc}	4.1 (EPI)
Bioconcentration Factor – BCF	2341 (EPI)
Persistence	
Probability of Rapid Biodegradation	Does not biodegrade fast (EPI)
Ultimate Biodeg Model	weeks – months (EPI)
Primary Biodeg Model	weeks (EPI)
Ready Biodegradability (MITI Model)	Not Ready Biodegradable (EPI)
Atmospheric Half-life	2 days [rxn with hydroxyl radicals] (EPI)
Hydrolysis Half-life	No hydrolyzable groups
Volatilization Half-life for Model River	8 hours (EPI)
Volatilization Half-life for Model Lake	9 days (EPI)
Removal in Sewage Treatment Plant* (Old Method)	90% (EPI)
Removal in Sewage Treatment Plant* (Draft Method)	>90% (EPI)
Experimental Biodeg Tests	None available
Byproducts	
Degradation Products	Not Assessed
Metabolites	Not Assessed

* Unless experimental data indicate otherwise, the maximum number used will be 90%

CAS No.	Submitter: SF Trainers, Inc.
ECOTOXICITY:	
ECOSAR Class	Neutral Organics
Acute Toxicity	
Fish LC_{50}	0.12 ppm, 96 hr (ECOSAR) (K_{ow} is above the cutoff for this effect)
Daphnid LC_{50}	0.097 ppm, 48 hr (ECOSAR) (K_{ow} is above the cutoff for this effect)
Green Algae EC_{50}	0.12 ppm, 96 hr (ECOSAR)
Chronic Toxicity	
Fish ChV	0.018 ppm (ECOSAR)
Daphnid ChV	0.024 ppm (ECOSAR)
Green Algae ChV	0.16 ppm (ECOSAR)
Overall Hazard Concern for Aquatic Toxicity	HIGH
Lowest Chronic COC (lowest ChV/10) – used as input to determine Aquatic Exposure in E-FAST	2 ppb (ECOSAR)
CANCER HEALTH EFFECTS:	
Experimental data	None identified
OncoLogic Results	Low-moderate based on halogenated nitroaromatics category
Overall Hazard Concern for Carcinogenicity	MODERATE
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	
Irritation	
Skin Sensitizer	
Reproductive Effects	
Developmental Effects	Moderate, based on analogy to 1,2-dichloro-4-nitrobenzene, which induced developmental effects in rats dosed via oral gavage. NOAEL = 10 mg/kg-day; LOAEL = 30 mg/kg-day (1).
Immune System Effects	
Neurotoxicity	
Genotoxicity	
Mutagenicity	
Systemic Effects	
Overall Hazard Concern for Non-Cancer Health Effects	HIGH

CAS No. N/A	**Submitter:** SF Trainers, Inc.

INDUSTRIAL OPERATIONS INFORMATION

Operation Name	Manufacturing	**Number of sites**	1
Location	Organic Chemicals Manufacture Plant	**Operating Days Per Year**	12

INDUSTRIAL RELEASE SUMMARY

Media	**Daily Release (kg/site-day)**	**Release Days per Year**	**No of Sites of Release**	**Total Annual Releases (kg/year -all sites)**	**Release site information (NPDES No. or SIC Code)**
Water	4 kg/site-day	12	1	48 kg/year	Organic Chemicals Manufacture

OCCUPATIONAL EXPOSURE SUMMARY

Route	**Dose Rate**	**Days/yr**	**Workers**	**Cancer LADD**	**Chronic ADD**	**Acute APDR**
Dermal	0.0015 mg/day	12	1	1.6×10^{-3} mg/kg-day	3.0×10^{-3} mg/kg-day	0.510 mg/kg-day
Inhalation	0.002 mg/day	12	1	2.2×10^{-2} mg/kg-day	6.0×10^{-1} mg/kg-day	0.599 mg/kg-day

Total number of Workers – All Sites	4

GENERAL POPULATION EXPOSURE SUMMARY

	Cancer LADDpot	**Chronic ADDpot**	**Acute ADRpot**
Drinking Water	2.03×10^{-6} mg/kg/day	3.80×10^{-6} mg/kg/day	3.56×10^{-3} mg/kg/day
Fish Ingestion	2.03×10^{-5} mg/kg/day	3.80×10^{-5} mg/kg/day	3.33×10^{-2} mg/kg/day
Fugitive Emissions	N/A	N/A	N/A
Incineration Emissions	N/A	N/A	N/A
Landfill Leaching	N/A	N/A	N/A
Dermal – Consumer Use	N/A	N/A	N/A
Inhalation – Consumer Use	N/A	N/A	N/A

AQUATIC EXPOSURE SUMMARY

Lowest Chronic COC – Aquatic Exposure	2 ug/L [ppb] (Fish/10)
Predicted Environmental Concentration (PEC)	74.0 ug/L [ppb]
PEC Exceeds Chronic COC (days / year)	9 days

RISK ASSESSMENT CALCULATIONS:

MOE – Acute Occupational Exposure	N/A
MOE – Chronic Occupational Exposure	16.7 (based on APDR for inhalation exposure and NOAEL for developmental toxicity)
MOE – Acute General Population Exposure	N/A
MOE – Chronic General Population Exposure	300 (based on ADRpot for fish ingestion exposure and NOAEL for developmental toxicity)

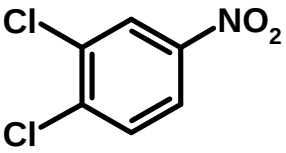
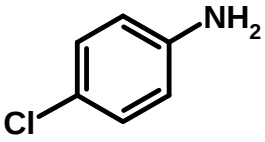
CONCLUSIONS:

Occupational Risk:
Risk of Non-Cancer Effects from Occupational Exposure: Potential for risk exists because the MOE < 100
Risk of Cancer Effects from Occupational Exposure: Potential for risk exists because cancer risk $>10^{-5}$

General Population Risk:
Risk of Non-Caner Acute Effects to General Population: N/A
Risk of Non-Cancer Chronic Effects to General Population: Low concern for risk because the MOE >100
Risk of Cancer Effects to General Population: Low concern for risk because cancer risk $<10^{-6}$

Aquatic Risk:
Acute Risk to the Aquatic Environment: Potential for risk exists because the PEC exceeds the acute COC
Chronic Risk to the Aquatic Environment: Low concern for risk because the PEC is exceeded by the chronic COC for less than 20 days per year.

Table I - Selected Analogs

Analog	Structure	Concern Identified	Basis of Concern	Concern Level	Reference
1,2-dichloro-4-nitrobenzene		**Developmental Toxicity**	Induced malformations in fetuses of orally treated rats at ≥30 mg/kg-day	**Moderate**	**Monsanto, 1990**
4-□hloroaniline		**Carcinogenicity**	Induced rare spleen neoplasms in male rats	**Moderate**	**NCI, 1979**

References

1. Monsanto Company; USEPA Status Report: Nitrated Orthene (1990), EPA Document No. 8EHQ-0590-0972, Fiche No. OTS0524331-1. Cited in HSDB, 2003.

2. HSDB (Hazardous Substances Data Bank). 2003. 3,4-DICHLORONITROBENZENE CASRN: 99-54-7. Available on-line at http://toxnet.nlm.nih.gov.

3. NCI (National Cancer Institute). 1979. Bioassay of p-chloroaniline for possible carcinogenicity. TR 189. Available on-line at http://ntp-server.niehs.nih.gov/htdocs/LT_rpts/tr189.pdf