

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 2):

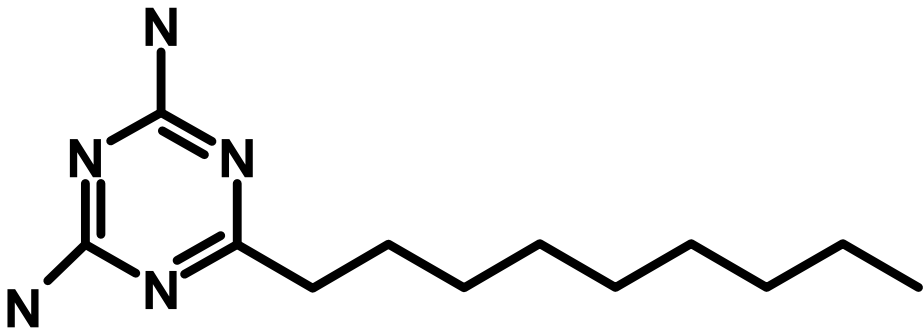
1,3,5-triazine-2,4-diamine, 6-nonyl

CAS Registry Number:

5921-65-3

Participant Name:

SF Trainers

Record ID: Training Session Example Chemical 2	CAS No. 5921-65-3
	MW: 237.35
	MF: C ₁₂ H ₂₃ N ₅
	Physical Form: Solid
	Submitter: SF Trainers, Inc.
	Trade Name: STICKTIGHT
	Use: An activator used in soldering flux for circuit boards
	Production Volume: 10,000 kg/yr

SMILES: n1c(nc(nc1N)CCCCCCCC)N

Name: 1,3,5-triazine-2,4-diamine, 6-nonyl-

Synonyms:

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?	NO		
Overall Hazard Concern	Human Health: Moderate Aquatic Toxicity: High		
Overall Risk Concern	Human Health: Low concern for risk Aquatic: Potential risk exists		

CAS No. 5921-65-3	Submitter: SF Trainers, Inc.
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	115-125 (exp, evaluated using 120 deg C as input for EPI)
Boiling Point (deg C)	392 (EPI)
Boiling Point Pressure (mm Hg)	760 (EPI)
Vapor Pressure (mm Hg)	1.45 x 10 ⁻⁶ (EPI)
Water Solubility	2.9 mg/L (EPI)
Octanol/Water Partition Coefficient - Log K _{ow}	4.15 (EPI)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC	5.7 x 10 ⁻⁹ atm-m ³ /mole (EPI)
Soil Adsorption Coefficient – Log K _{oc}	3.6 (EPI)
Bioconcentration Factor – BCF	3.3 (EPI)
Persistence	
Probability of Rapid Biodegradation	Does not biodegrade fast (EPI)
Ultimate Biodeg Model	weeks-months (EPI)
Primary Biodeg Model	days-weeks (EPI)
Ready Biodegradability (MITI Model)	Not Ready Biodegradable (EPI)
Atmospheric Half-life	11 hours [rxn with hydroxyl radicals] (EPI)
Hydrolysis Half-life	Not Available
Volatilization Half-life for Model River	18 years, essentially non-volatile from water (EPI)
Volatilization Half-life for Model Lake	200 years, essentially non-volatile from water (EPI)
Removal in Sewage Treatment Plant* (Old Method)	37% (EPI)
Removal in Sewage Treatment Plant* (Draft Method)	73% (EPI)
Experimental Data	
Byproducts	
Degradation Products	Not Assessed
Metabolites	Not Assessed

* Unless experimental data indicate otherwise, the maximum value used by EPA will be 90% removal.

CAS No. 5921-65-3	Submitter: SF Trainers, Inc.
ECOTOXICITY:	
ECOSAR Class	Anilines (unhindered), Anilines (amino-meta), Triazines (aromatic)
Acute Toxicity	
Fish LC ₅₀	1.1 ppm, 96-hr (ECOSAR, Anilines (unhindered))
Daphnid LC ₅₀	0.106 ppm, 48-hr (ECOSAR, Anilines (amino-meta))
Green Algae EC ₅₀	0.022 ppm, 96-hr (ECOSAR, Triazines (aromatic))
Chronic Toxicity	
Fish ChV	0.005 ppm (ECOSAR, Anilines (unhindered))
Daphnid ChV	0.006 ppm (ECOSAR, Anilines (amino-meta))
Green Algae ChV	0.021 ppm (ECOSAR, Triazines (aromatic))
Overall Hazard Concern for Aquatic Toxicity	HIGH: Acute and chronic effects
Lowest Chronic COC (lowest ChV/10) – used as input to determine Aquatic Exposure in E-FAST	1 ug/L (ppb) (ECOSAR)
CANCER HEALTH EFFECTS:	
Experimental data	Melamine has been shown to induce tumors via stone formation (1)
OncoLogic Results	Low concern predicted based on the aromatic amines category; marginal concern was assigned to melamine based on specific evaluation in OncoLogic
Overall Hazard Concern for Carcinogenicity	LOW
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Oral LD50 values for the submitted substance range from ~3000 to 7000 mg/kg (2)
Irritation	The structural analog melamine produced very slight irritation in laboratory animals and no irritation in a human patch test (3).
Skin Sensitizer	The structural analog melamine did not induce skin sensitization in humans (3).
Reproductive Effects	No reproductive toxicity tests were located; however, the structural analog melamine did not affect reproductive tissues in oral subchronic and chronic tests in rats and mice (1).
Developmental Effects	The structural analog melamine did not cause developmental toxicity in rats administered via i.p. injection at up to 70 mg/kg-day (5).
Immune System Effects	No immune toxicity tests were identified; however, the structural analog melamine did not affect immune system tissues in oral subchronic and chronic tests in rats and mice (1)
Genotoxicity	The structural analog melamine tested negative in an unscheduled DNA synthesis test (4)
Mutagenicity	The structural analog melamine tested negative in an Ames test (+/- S9) and a sex-linked recessive lethal mutation test in <i>Drosophila</i> (4).
Systemic Effects	Moderate, based on analogy to melamine, which has been shown to affect the urinary bladder in rats and mice in subchronic and chronic studies. Effects have included ulceration, stone formation, and tumor formation. Tumor formation, however, has been shown to be a secondary effect caused by test-substance crystallization and stone formation in urinary bladder. LOAEL ~ 112.5 mg/kg-day; NOAEL ~ 50 mg/kg-day (1).
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE

CAS No. 5921-65-3				Submitter: SF Trainers, Inc.		
INDUSTRIAL OPERATIONS INFORMATION						
Operation Name		Manufacturing		Number of sites		1
Location		Organic Chemicals Manufacture Plant		Operating Days Per Year		25
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	2 kg/day	25	1	50 kg/year	Organic Chemicals Manufacture	
OCCUPATIONAL EXPOSURE SUMMARY						
Route	Dose Rate	Days/yr	# Workers	Cancer LADD	Chronic ADD	Acute APDR
Dermal	0.001	25	1	1.8×10^{-3} mg/kg-day	2.1×10^{-3} mg/kg-day	6.8×10^{-2} mg/kg-day
Inhalation	0.0012	25	1	4.1×10^{-4} mg/kg-day	6.2×10^{-4} mg/kg-day	7.2×10^{-3} mg/kg-day
Total number of Workers – All Sites				1		
GENERAL POPULATION EXPOSURE SUMMARY						
	Cancer LADDpot		Chronic ADDpot		Acute ADRpot	
Drinking Water	5.70×10^{-6} mg/kg-day		1.07×10^{-5} mg/kg-day		4.81×10^{-3} mg/kg-day	
Fish Ingestion	8.07×10^{-8} mg/kg-day		1.51×10^{-7} mg/kg-day		6.33×10^{-5} 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				1 ug/L (ppb)		
Predicted Environmental Concentration (PEC)				99.8 ug/L (ppb)		
PEC Exceeds Chronic COC (days / year)				23 days/yr		
RISK ASSESSMENT CALCULATIONS:						
MOE – Acute Occupational Exposure				N/A		
MOE – Chronic Occupational Exposure				2.4×10^4 (based on occupational dermal exposure and NOAEL for systemic toxicity)		
MOE – Acute General Population Exposure				N/A		
MOE – Chronic General Population Exposure				2.6×10^6 (based on drinking water exposure and NOAEL for systemic toxicity)		

CONCLUSIONS:

Occupational Risk:

Risk of Non-Cancer Effects from Occupational Exposure: Low concern for risk because the MOE > 100

General Population Risk:

Risk of Non-Cancer Acute Effects to the General Population: N/A

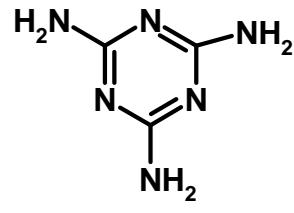
Risk of Non-Cancer Chronic Effects to the General Population: Low concern for risk because MOE >100

Aquatic Risk:

Risk of Acute Effects to the Aquatic Environment: Potential for acute aquatic risk exists because the PEC is greater than the acute COC.

Risk of Chronic Effects to the Aquatic Environment: Potential for chronic aquatic risk exists because the PEC exceeds the COC for more than 20 days per year.

Table I - Selected Analogs

Analog	Structure	Concern Identified	Basis of Concern	Concern Level	Reference
Melamine		Systemic toxicity	Urinary bladder effects in rats and mice exposed in the diet in subchronic and chronic tests. LOAEL ~ 112.5 mg/kg-day; NOAEL ~ 50 mg/kg-day	Moderate	NTP, 1983

References

1. NTP (National Toxicology Program). 1983. Toxicology and Carcinogenesis Studies of Melamine (CAS No. 108-78-1) in F344/N Rats and B6C3F1 Mice (Feed Study). Technical Report Series No. 245. U.S. Department of Health and Human Services. National Institutes of Health.
2. NTP. 2003. Health and Safety report for melamine. Available on-line at <http://ntp-server.niehs.nih.gov>
3. Clayton, G. D. and F. E. Clayton (eds.). Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology. 3rd ed. New York: John Wiley Sons, 1981-1982. 2772 (Cited in HSDB).
4. IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Man. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work).p. V39 341. (Cited in HSDB, 2003)
5. IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Man. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work).p. V39 340 (1986).
6. HSDB (Hazardous Substances Data Bank). 2003. Melamine. Available on-line at <http://toxnet.nlm.nih.gov>.