

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY WASHINGTON, D.C. 20460

OFFICE OF PREVENTION, PESTICIDES AND TOXIC SUBSTANCES

March 17, 2005

ACTION MEMORANDUM

- SUBJECT: Inert Ingredient Tolerance Reassessment Phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt
- FROM: Dan Rosenblatt, Chief Minor Use, Inerts, and Emergency Response Branch
- TO: Lois A. Rossi, Director Registration Division

I. FQPA REASSESSMENT ACTION

Action: Reassessment of one (1) inert ingredient exemption from the requirement of a tolerance.

Chemical and Use Summary: See table below.

Tolerance Exemption Being Reassessed						
Tolerance Exemption Expression	CAS Reg No.	40 CFR §	Use (Pesticidal)	List Classification		
Phenolsulfonic acid- formaldehyde-urea condensate and its sodium salt	29405-16-1 [Benzenesulfonic acid, 4-hydroxy-, polymer with formaldehyde and urea (9CI)]	180.920 ^{1/} id, nd	Dispersant			
	9041-04-7 [Benzenesulfonic acid, hydroxy-, polymer with formaldehyde and urea (9CI)]					

71608-70-3 [Benzenesulfonic acid, 4-hydroxy-, polymer with formaldehyde and urea, sodium salt (9CI)]		
52277-29-9 [Benzenesulfonic acid, hydroxy-, polymer with formaldehyde and urea, sodium salt (9CI)]		3

List Reclassification Determination: Phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt is classified as a List 3 inert ingredient (under CAS Reg. No. 52277-29-9) and is uncategorized as to list classification status under CAS Reg. Nos. 29405-16-1, 9041-04-7, and 71608-70-3. Based on the low risk and low toxicity findings, phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt (under each of the CAS Reg. Nos. noted above) can be reclassified as a List 4A inert ingredient.

II. MANAGEMENT CONCURRENCE

I concur with the reassessment of the one (1) exemption from the requirement of a tolerance for the inert ingredient phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt, and with the List reclassification determination, as described above. I consider the one (1) exemption from the requirement of a tolerance for phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt adenosine established in 40 CFR §180.920 [formerly 40 CFR§180.1001(d)] to be reassessed as of the date of my signature, below. A Federal Register Notice regarding this tolerance exemption reassessment decision will be published in the near future.

Lots A. Rossi, Director Registration Division

3/22/05 Date:

cc: Debbie Edwards, SRRD Joe Nevola, SRRD



UNITED STATES ENVIRONMENTAL PROTECTION AGENCY WASHINGTON, D.C. 20460

OFFICE OF PREVENTION, PESTICIDES AND TOXIC SUBSTANCES

March 17, 2005

MEMORANDUM

SUBJECT: Reassessment of the Exemption from the Requirement of a Tolerance for Phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt $2 \circ 10^{-10}$

FROM:	Kerry Leifer, Inerts Team Leader Minor Use, Inerts and Emergency Response Branch Registration Division (7505C)
	Registration Division (7505C)

- THRU: Pauline Wagner Resistration Division (7505C)
- TO: Dan Rosenblatt, Chief Minor Use, Inerts and Emergency Response Branch Registration Division (7505C)

Background

Attached is the science assessment for phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt. This assessment summarizes available information on the use, physical/chemical properties, toxicological effects, exposure profile, and environmental fate and ecotoxicity of phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt. The purpose of this document is to reassess the existing exemption from the requirement of a tolerance for residues of phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt as required under the Food Quality Protection Act (FQPA).

Executive Summary

This report evaluates phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt, a pesticide inert ingredient for which an exemption from the requirement of a tolerance

exists for its residues when used in pesticide formulations applied to growing crops only under 40 CFR §180.920 [formerly 40 CFR §180.1001(d)] for use as a dispersant.

A structure activity relationship analysis of phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt was conducted by the Office of Pollution Prevention and Toxics (OPPT) Structure Activity Team. The OPPT assessment concluded that phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt was poorly absorbed via all routes of exposure and is of low concern for human health effects, with no identified health concerns. Phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt is water soluble and does not undergo ready biodegradation, however due to its strong sorption to soils/sediments and negligible migration to ground water, it would not be expected to be present in drinking water while also being of low concern for toxicity to aquatic organisms.

Taking into consideration all available information on phenolsulfonic acid-formaldehydeurea condensate and its sodium salt, it has been determined that there is a reasonable certainty that no harm to any population subgroup will result from aggregate exposure to phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt when considering dietary exposure and all other non-occupational sources of pesticide exposure for which there is reliable information. Therefore, it is recommended that the exemption from the requirement of a tolerance established for residues of phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt in/on raw agricultural commodities can be considered reassessed as safe under section 408(q) of the FFDCA.

I. <u>Introduction</u>

This report evaluates phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt, a pesticide inert ingredient for which an exemption from the requirement of a tolerance exists for its residues when used in pesticide formulations applied to growing crops only under 40 CFR §180.920 [formerly 40 CFR §180.1001(d)].

Phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt is a copolymer of phenolsulfonic acid (or the sodium salt of phenolsulfonic acid) with formaldehyde and urea. This phenolic-type thermoset resin is a polymer that is formed when formaldehyde condenses with phenolsulfonic acid and urea, thereby forming a number of repeating units of phenolsulfonic acid and urea linked via a methylene (-CH₂-) group, with the molecular weight of the polymer being determined by the number of monomeric units. Phenolic resins are generally brittle solids with Bakelite (phenolsulfonic acid-formaldehyde condensate) being one of the first plastics widely used in the consumer market (Fadem, 1996).

II. <u>Use Information</u>

Pesticides

The tolerance exemption for the inert ingredient phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt is given in Table 1 below.

Table 1. Tolerance Exemption Being Reassessed in this Document						
Tolerance Exemption Expression	CAS Reg No.	40 CFR §	Use (Pesticidal)	List Classification		
Phenolsulfonic acid- formaldehyde-urea condensate and its sodium salt	29405-16-1 [Benzenesulfonic acid, 4-hydroxy-, polymer with formaldehyde and urea (9CI)]	180.920 ^{1/}	Dispersant			
	9041-04-7 [Benzenesulfonic acid, hydroxy-, polymer with formaldehyde and urea (9CI)]					
	71608-70-3 [Benzenesulfonic acid, 4-hydroxy-, polymer with formaldehyde and urea, sodium salt (9CI)]					
	52277-29-9 [Benzenesulfonic acid, hydroxy-, polymer with formaldehyde and urea, sodium salt (9CI)]			3		

1. Residues listed in 40 CFR §180.920 [formerly 40 CFR§ 180.100(d)] are exempted from the requirement of a tolerance when used as inert ingredients in pesticide formulations when applied to growing crops only.

Other Uses

No other use information was available for phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt.

III. <u>Physical and Chemical Properties</u>

A representative chemical structure and some physical and chemical characteristics of phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt are found in Appendix A.

IV. Hazard Assessment

A. Hazard Profile

A structure activity relationship analysis of phenolsulfonic acid-formaldehyde-urea condensate, sodium salt, was conducted by the Office of Pollution Prevention and Toxics (OPPT) Structure Activity Team. The OPPT assessment concluded that phenolsulfonic acid-formaldehyde-urea condensate, sodium salt, is of low concern for human health, with no significant identified health concerns. The full OPPT Structure Activitity Team report for phenolsulfonic acid-formaldehyde-urea condensate, sodium salt, sodium salt is contained in Appendix A.

B. Toxicological Data

No references to toxicity studies on phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt were identified in the open literature.

C. Metabolism And Pharmacokinetics

The OPPT Structure Activity Team assessment noted that there is no absorption of phenolsulfonic acid-formaldehyde-urea condensate, sodium salt, through the skin for all possible molecular weight material. Absorption of low molecular weight (molecular weight less than 1000) material is poor through the gastrointestinal (GI) tract and good through the lungs. There is no adsorption of high molecular weight material (molecular weight greater than 10,000) through the lungs and GI tract. Any material of molecular weight greater than 1000 and less than 10,000 is expected to have no absorption through the GI tract and moderate absorption through the lungs (Appendix A).

D. Special Considerations for Infants and Children

Phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt is of low concern for human health effects, therefore a safety factor analysis has not been used to assess the risks resulting from the use of phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt and an additional tenfold safety factor for the protection of infants and children is unnecessary.

V. <u>Exposure Assessment</u>

Phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt is not absorbed through the skin, with adsorption being poor to nil through the GI tract, therefore no further exposure assessment via these routes of exposure is necessary. Absorption of lower molecular weight species of phenolsulfonic acid-formaldehyde-urea condensate, sodium salt is expected to be moderate to good through the lungs, however, since no there are no identified health concerns associated with inhalation exposure to phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt, no further inhalation exposure assessment is necessary.

VI. <u>Aggregate Exposures</u>

In examining aggregate exposure, FFDCA section 408 directs EPA to consider available information concerning exposures from the pesticide residue in food and all other non-occupational exposures, including drinking water from ground water or surface water and exposure through pesticide use in gardens, lawns, or buildings (residential and other indoor uses).

For phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt, a qualitative assessment for all pathways of human exposure (food, drinking water, and residential) is appropriate given the lack of human health concerns associated with exposure to phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt.

VII. <u>Cumulative Exposure</u>

Section 408(b)(2)(D)(v) of the FFDCA requires that, when considering whether to establish, modify, or revoke a tolerance, the Agency consider "available information" concerning the cumulative effects of a particular pesticide's residues and "other substances that have a common mechanism of toxicity."

Unlike other pesticides for which EPA has followed a cumulative risk approach based on a common mechanism of toxicity, EPA has not made a common mechanism of toxicity finding as to phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt and any other substances and this material does not appear to produce a toxic metabolite produced by other substances. For the purposes of this tolerance action, therefore, EPA has not assumed that phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt has a common mechanism of toxicity with other substances. For information regarding EPA's efforts to determine which chemicals have a common mechanism of toxicity and to evaluate the cumulative effects of such chemicals, see the policy statements released by EPA's Office of Pesticide Programs concerning common mechanism determinations and procedures for cumulating effects from substances found to have a common mechanism on EPA's website at http://www.epa.gov/pesticides/cumulative/

VIII. Environmental Fate Characterization/Drinking Water Considerations

Phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt is water soluble and does not undergo ready biodegradation, however due to its strong sorption to soils/sediments and negligible migration to ground water, it would not be expected to be present in drinking water sources as a result of its use as a pesticide inert ingredient. Estimated environmental fate properties of phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt are given in Appendix A.

IX. Human Health Risk Characterization

Based upon the OPPT Structure Activity Team's structure activity relationship analysis, phenolsulfonic acid-formaldehyde-urea condensate, sodium salt is of low concern for human health effects. Phenolsulfonic acid-formaldehyde-urea condensate, sodium salt, is not expected to be absorbed by the skin with poor or no absorption occurring via the GI tract. Absorption of phenolsulfonic acid-formaldehyde-urea condensate, sodium salt, in lungs is expected to be moderate to good for lower molecular weight species, but no identifiable toxicological endpoints are associated with inhalation exposure to phenolsulfonic acid-formaldehyde-urea condensate, sodium salt.

Taking into consideration all available information on phenolsulfonic acid-formaldehyde- urea condensate and its sodium salt, it has been determined that there is a reasonable certainty that no harm to any population subgroup will result from aggregate exposure to phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt when considering dietary exposure and all other non-occupational sources of pesticide exposure for which there is reliable information. Therefore, it is recommended that the exemption from the requirement of a tolerance established for residues of phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt in/on raw agricultural commodities can be considered reassessed as safe under section 408(q) of the FFDCA.

X. Ecotoxicity and Ecological Risk Characterization

There are no available aquatic toxicity studies on phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt (ECOTOX, 2002), however, as part of its evaluation of phenolsulfonic acid-formaldehyde-urea condensate, sodium salt, the OPPT Structure Activity Team rated phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt as moderate concern for toxicity to fish, algae, and aquatic invertebrates with a concern concentration in water of 30 ppb (Appendix A). There are no concerns from risks to aquatic organisms associated with the use of phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt when used as an inert ingredient as, based on its environmental fate characterization (see section VIII above), it would not be expected to be present in surface water at levels at or near the concern concentration of 30 ppb.

References:

ECOTOX. 2002. U.S. Environmental Protection Agency. 2002. ECOTOX User Guide: ECOTOXicology Database System. Version 3.0. <u>http://www.epa.gov/ecotox/</u> Search terms: CAS Reg Nos: 139-44-6 (February 14, 2005) Fadem, L. and Fadem, S.Z. 1996. Bakelite: A Revolutionary Early Plastic. http://www.deco-echoes.com/bakelite.html

OPPT. 2004. Office of Pollution Prevention and Toxics Structure Activity Team Report: Benzenesulfonic acid, 4-hydroxy, polymer with formaldehyde and urea, sodium salts. December 14, 2004

APPENDIX A

OPPT SAT Review of Phenolsulfonic acid-formaldehyde-urea condensate and its sodium salt

~			ver. 04/98	CBI7 (YES/NU))	
Case #:	Z-05-0009		DCN:		
SAT Date:	12/14/2004		SAT Chair:	Beckie Jone	S
Submitter:		······································			
Chemical Name	ə:		<u></u>		
Benzenesulfo	nic acid, 4-hvdro	oxy-, polymer w	ith formaldeh	vde and urea. sodium	salts
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CAS RN:			Trade Name:		
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71608-70-3

ECOTOX

2

STRUCTURE ACTIVITY TEAM REPORT

CASE NUMBER: 205-0009

RELATED CASES:

.

CONCLUSIONS/DISCUSSIONS

TYPE OF CONCERN:

LEVEL OF CONCERN:

KEYWORDS:

AQUATOX-A,C

SUMMARY OF ASSESSMENT

FATE: Solid S (25°C) > 100 g/L(Analogs); VP@25C(mm) < 1.0E-6(E); H < 1.00E-8(E) POTW removal (%) = 50-90 via sorption Time for complete ultimate aerobic biodeg > mo PBT Potential: P3B1T1 Sorption to soils/sediments = v.strong *CEB FATE: Migration to ground water = negl

HEALTH

1

HEALTH: Absorption is nil through the skin for all possible molecular weight material. Absorption of low molecular weight material (<1000) is poor through the GI tract and good through the lungs. Absorption of high molecular weight material (>10,000) is nil through the lungs and GI tract. Any material that is between these two ranges (< 10,000 and >1000) is expected to have nil absorption through the GI tract but moderate absorption through the lungs. No significant health concerns. *CEB HEALTH: Low concern.

ECOTOX: Predicted (P) and measured (M) toxicity values in mg/L (ppm) are: fish 96-h LC50 2.0 Ρ > daphnid 48-h LC50 2.0 ₽ > green algal 96-h EC50 c > 2.0 ₽ fish chronic value 0.310 P > daphnid ChV 0.310 P > algal ChV 0.500 P > Predictions are based on SAR-nearest analog analysis for poly[aromatic sulfonated phenols] page 207 in Boethling RS and Nabholz JV. 1997. Chapter 10. Environmental Assessment of Polymers under the US Toxic Substances Control Act, pages 187 to 234 in Hamilton JD and Sutcliffe R (eds) Ecological Assessment of Polymers, Van Nostrand Reinhold New York); SAR chemical class = polymer-anionic-aromatic sulfonated phenols; MW>621 with ?* <1000 and ?% <500; pH7; effective concentrations based on 100%</pre>

active ingredients and mean measured concentrations; hardness <150.0 mg/L as CaCO3; and TOC <2.0 mg/L; moderate concern for toxicity assessment factor = 10.0 concern concentration = 0.030 mg/L (ppm) *CEB ECOTOX: All releases to water with CC = 30 ppb

Becky Jones 564-8919

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PMN:	Z-05-00	009	CAS RN:		г	
Chemical Name: Benzenesulfonic	acid 4-hydroxy	- polymer with for	maldehyde and urea, s	odium	Analogs	:
benzentesationie		salts			Producti	on Volume:
Structure:						
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Use: Pesticide inert ingr Formula: Mol Weight: MP: H2O Sol (g/L): Endpoint (mg/L) Fish 96-h Daphnid 48-h Algal 96-h Fish ChV Daphnid ChV Algal ChV BCF CHEMICAL CLAS	redient. $C_{19}H_{22}N_6Na_2$ Est. Value $\overrightarrow{200}$	O ₁₁ S ₂ >100Phy Meas. Value	Eq Wt: 620.53 Wt%<500: BP: rsical State: Comments Poly por Orfenci Annatio	Left rh - hls	Solid Solid actas aconat nã on	Wt%<1000 VP: Log P:-4,9 an dr glouds ta pelfor ta pelfor d - (b)
Use: Pesticide inert ingr Formula: Mol Weight: MP: H2O Sol (g/L): Endpoint (mg/L) Fish 96-h Daphnid 48-h Algal 96-h Fish ChV Daphnid ChV Algal ChV BCF CHEMICAL CLAS ECOTOX CONCE	redient. C ₁₉ H ₂₂ N ₆ Na ₂ Est. Value >2.0 >2.0 >0.3 00 SS: ERN H M	SAR:	Eq Wt: 620.53 Wt%<500: BP: sical State: Comments <i>Polyper</i> <i>Orfenci</i> <i>Annatic</i> <i>Mannatic</i> <i>Mannatic</i> <i>Mannatic</i> <i>Mannatic</i> <i>Mannatic</i>	ento mon	Solid relas aronat with our	Wt%<1000 VP: Log P:-4.9 ar dr plands ta follor d - (10)



 ${\tt SMILES} : {\tt NC(=0) \ NCc1cc} ({\tt S(=0) \ (=0) \ 0}) \ cc \ ({\tt c10}) \ CNC \ (=0) \ NCN \ (C(=0) \ N) \ Cc2c \ (0) \ ccc \ (c2) \ S \ (0) \ (=0) \ Cc2c \ (0) \ ccc \ (c2) \ S \ (0) \ (=0) \ Cc2c \ (0) \ ccc \ (c2) \ S \ (0) \ (=0) \ Cc2c \ (0) \ ccc \ (c2) \ S \ (0) \ (=0) \ Cc2c \ (0) \ ccc \ (c2) \ S \ (0) \ (=0) \ Cc2c \ (0) \ ccc \ (c2) \ S \ (0) \ (=0) \ Cc2c \ (0) \ ccc \ (c2) \ S \ (0) \ (=0) \ Cc2c \ (0) \ ccc \ (c2) \ S \ (0) \ (=0) \ Cc2c \ (0) \ ccc \ (c2) \ S \ (0) \ (=0) \ Cc2c \ (0) \ ccc \ (c2) \ S \ (0) \ (=0) \ Cc2c \ (0) \ ccc \ (c2) \ S \ (0) \ (=0) \ Cc2c \ (0) \ ccc \ (c2) \ S \ (0) \ (=0) \ Cc2c \ (0) \ ccc \ (c2) \ S \ (0) \ (=0) \ Cc2c \ (0) \ ccc \ (c2) \ S \ (0) \ (=0) \ Cc2c \ (0) \ ccc \ (c2) \ S \ (0) \ (=0) \ Cc2c \ (0) \ ccc \ (c2) \ S \ (0) \ (=0) \ Cc2c \ (0) \ ccc \ (c2) \ S \ (0) \ (=0) \ Cc2c \ (0) \ ccc \ (c2) \ S \ (0) \ (=0) \ Cc2c \ (c2) \ S \ (0) \ (=0) \ Cc2c \ (c2) \ S \ (0) \ (=0) \ Cc2c \ (c2) \ S \ (c2) \ Cc2c \ (c2) \ S \ (c2) \ Cc2c \ (c2) \ S \ (c2) \ (c2) \ Cc2c \ (c2) \ S \ (c2) \ (c2) \ Cc2c \ (c2) \ S \ (c2) \ (c2) \ Cc2c \ (c2) \ S \ (c2) \ (c2) \ Cc2c \ (c2) \ S \ (c2) \ (c2) \ Cc2c \ (c2) \ S \ (c2) \$ 0)0

CHEM : CAS Num: ChemID1: ChemID2: ChemID2: ChemID3: MOL FOR: C19 H26 N6 Oll S2 MOL WT : 578.57 Log Kow: -4.87 (User entered) Melt Pt: 100.00 deg C Wat Sol: 1.523E+010 mg/L (calculated)

ECOSAR v0.99h Class(es) Found

Neutral Organics-acid Phenols-acid Ureas(substituted)-acid

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ECOSAR Class	Organism	Duration	End Pt	ma/L (p	ed nm)
				=======	===
Neutral Organic SAR : (Baseline Toxicity)	Fish	14-day	LC50	7.48e+00	8

--> Acid moeity found: Predicted values multiplied by 10

Neutral Org	anics-acid	:	Fish	96-hr	LC50	1.23e+010
Neutral Or	janics-acid	:	Fish	14-day	LC50	7.48e+009
Neutral Org	anics-acid	:	Daphnid	48-hr	LC50	8.2e+009
Neutral Org	anics-acid	:	Green Algae	96-hr	EC50	3.45e+009
Neutral Ord	anics-acid	:	Fish	30-day	ChV	5.24e+008
Neutral Ord	anics-acid	:	Daphnid	16-day	EC50	2.08e+007
Neutral Orc	anics-acid	:	Green Algae	96-hr	ChV	6.52e+006
Neutral Ord	anics-acid	:	Fish (SW)	96-hr	LC50	1.02e+008
Neutral Ord	anics-acid	:	Mysid Shrimp	96-hr	LC50	4.78e+011 *
Neutral Org	janics-acid	:	Earthworm	14-day	LC50	4.65e+006
Phenols-aci	d	:	Fish	96-hr	LC50	1.45e+007
Phenols-aci	d	:	Daphnid	48-hr	LC50	2.01e+005
Phenols-aci	d	:	Green Algae	96-hr	EC50	3.45e+009
Phenols-aci	d	:	Fish	30-day	ChV	2.54e+006
Phenols-aci	ld	:	Fish	90-day	ChV	8132.942
Phenols-aci	d	:	Daphnid	21-day	ChV	1.51e+006
Phenols-aci	d	:	Green Algae	96-hr	ChV	6.52e+006
Ureas (subst	ituted)-acid	:	Algae	4-hr	EC50	1.51e+010

Ureas(substituted)-acid : Algae

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect. Neutral Organics: Neutral organics: Fish and daphnid acute toxicity log Kow cutoff: 5.0 Green algal EC50 toxicity log Kow cutoff: 6.4 Chronic toxicity log Kow cutoff: 8.0 MW cutoff: 1000 Phenols: Fich and is held Fish and daphnid acute toxicity log Kow cutoff: 7.0

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CHEMICAL:	Unknown	1	14:26:23 12	2/13/:4
MOL WT : 5	576.58			
MOL FOR: 0	C19H24N6	5011S2		
SMILES : N	VC (=0) NC	Cc1cc(S(=0)(=0)0)cc(c10)CNC(=0)NCN(C(=(=0)NC)NC(=(=)NCN(C(=0)NC)NC(=()NC)NC)))))))))))))))))))))))))	1) Cc2c (0) ccc	c(c2)S(=
ISOC-ID: -	2	Za-aaAaa-aZA	Za-aaaa	a-a
FRAG-ID: 1	L11_1	2_2_2_23_44_4_4_5_5_5_5	56	7
H-COUNT: 2	212	$2 _ 1 _ _ 1 _ 1 _ 1 _ 21 _ 12 _ 22$	$2_2_11_1$	1
SMILES : () (=0)0			
ISUC-ID:	7 7 7			
H-COINT	′ <u> </u>			
	4		L	
Class	Туре	Contribution Description	Comment	Value
	+		+	
FRAGMENT	#1	NH-Urea	MEASURED	-1.710
FRAGMENT	#2	Sulfonic acid	MEASURED	-1.630
FRAGMENT	#3	Alcohol or Hydroxy	MEASURED	-0.440
FRAGMENT	#4	N, N'Urea	APPROX.	-1.980
FRAGMENT	# 5	N, N-Urea	A PRIORI	-3.300
FRAGMENT	# 6 # 7	Alconol or Hydroxy	MEASURED	-0.440
FRAGMENT		Sullonic acid	MEASURED	-1.630
ISOLATING	CARBON	4 Allphatic isolating carbon(s)		0.780
ISOLATING	CARBON	12 Aromatic isolating carbon(s)		1.560
EXFRAGMENT	HIDROG	13 Hydrogen(s) on isolating carbons		2.951
EXFRAGMENT	BONDS	6 chain and 0 alicyclic (net)		-0.720
PROXIMITY	1-0-1	rrags 4 and 5:32 (-1.980+ -3.300)		1.690
RESULT	v3.3	Benzyl approx. based on a priori value	ESTIMATE	-4.869
	+		+	

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ChemIDplus

National L Speciali	Aboet · Contact · Search Ibrary of Medicine zed Information Services
ChemIDplus Lite	Tox. & Env. Health > TOXNET > Return to Results Page
Full Record	and A hydroxy, nolymor with formal dehydo and yroa
Benzenesunome	sodium salt RN: 71608-70-3
Names and Synonyms	Systematic Name Description acid, 4-hydroxy-, polymer with formaldehyde and urea, sodium salt
Registry Numbers	CAS Registry Number I 71608-70-3
	System Generated Number
Classification Codes	Classification Code ISCA Flag: XU [Exempt from reporting under IUR]
Formulas	Molecular Formula ᆁ (C6-H6-O4-S.C-H4-N2-O.C-H2-O)xx-Na
	Molecular Formula Fragments
	İ C-H4-N2-O
	I COMPONENT I Na
Locators	File Locator
	Internet Locator I EPA CRS
U.S. Na Nat Cop	ational Library of Medicine, 8600 Rockville Pike, Bethesda, MD 20894, ional Institutes of Health. Department of Health & Human Services yright and Privacy Policy. Freedom of Information Act. Accessibility Customer Service: tehip@teh.nlm.nih.gov. Last modified on September 9, 2004.

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