

SCREENING-LEVEL HAZARD CHARACTERIZATION

Fatty Nitrogen Derived (FND) Ether Amines Category 1

SPONSORED CHEMICALS

1-Propanamine, 3-(C₈₋₁₀-alkyloxy) derivatives	CASRN 68784-38-3
1-Propanamine, 3-(isodecyloxy)-	CASRN 30113-45-2
1-Propanamine, 3-(C₉₋₁₁-isoalkyloxy) derivs., C₁₀ rich	CASRN 218141-16-3
1-Propanamine, 3-(C₁₁₋₁₄-isoalkyloxy) derivs., C₁₃ rich	CASRN 151789-06-9
1,3-Propanediamine, N-[3-(tridecyloxy)propyl]-, branched	CASRN 68479-04-9
1,3-Propanediamine, N-(3-(C₁₁₋₁₄-isoalkyloxy)propyl) derivs., C₁₃ rich	CASRN 151789-07-0

SUPPORTING CHEMICALS

1-Propanamine, 3-(isodecyloxy)-, acetate	CASRN 28701-67-9
1-Propanamine, 3-(tridecyloxy)-, branched	CASRN 68511-40-0
1-Dodecanamine, N,N-dimethyl-	CASRN 112-18-5
1-Hexadecanamine, N,N-dimethyl-	CASRN 112-69-6
cis-9-Octadecylamine	CASRN 112-90-3
1-Octadecanamine, N,N-dimethyl-	CASRN 124-28-7
N-coco alkyl derivatives of 2,2'-iminobis ethanol	CASRN 61791-31-9

The High Production Volume (HPV) Challenge Program¹ was conceived as a voluntary initiative aimed at developing and making publicly available screening-level health and environmental effects information on chemicals manufactured in or imported into the United States in quantities greater than one million pounds per year. In the Challenge Program, producers and importers of HPV chemicals voluntarily sponsored chemicals; sponsorship entailed the identification and initial assessment of the adequacy of existing toxicity data/information, conducting new testing if adequate data did not exist, and making both new and existing data and information available to the public. Each complete data submission contains data on 18 internationally agreed to "SIDS" (Screening Information Data Set^{1,2}) endpoints that are screening-level indicators of potential hazards (toxicity) for humans or the environment.

The Environmental Protection Agency's Office of Pollution Prevention and Toxics (OPPT) is evaluating

¹ U.S. EPA. High Production Volume (HPV) Challenge Program; <http://www.epa.gov/chemrtk/index.htm>.

² U.S. EPA. HPV Challenge Program – Information Sources; <http://www.epa.gov/chemrtk/pubs/general/guidocs.htm>.

the data submitted in the HPV Challenge Program on approximately 1400 sponsored chemicals by developing hazard characterizations (HCs). These HCs consist of an evaluation of the quality and completeness of the data set provided in the Challenge Program submissions. They are not intended to be definitive statements regarding the possibility of unreasonable risk of injury to health or the environment.

The evaluation is performed according to established EPA guidance^{2,3} and is based primarily on hazard data provided by sponsors; however, in preparing the hazard characterization, EPA considered its own comments and public comments on the original submission as well as the sponsor's responses to comments and revisions made to the submission. In order to determine whether any new hazard information was developed since the time of the HPV submission, a search of the following databases was made from one year prior to the date of the HPV Challenge submission to the present: (ChemID to locate available data sources including Medline/PubMed, Toxline, HSDB, IRIS, NTP, ATSDR, IARC, EXTOXNET, EPA SRS, etc.), STN/CAS online databases (Registry file for locators, ChemAbs for toxicology data, RTECS, Merck, etc.) and Science Direct. OPPT's focus on these specific sources is based on their being of high quality, highly relevant to hazard characterization, and publicly available.

OPPT does not develop HCs for those HPV chemicals which have already been assessed internationally through the HPV program of the Organization for Economic Cooperation and Development (OECD) and for which Screening Initial Data Set (SIDS) Initial Assessment Reports (SIAR) and SIDS Initial Assessment Profiles (SIAP) are available. These documents are presented in an international forum that involves review and endorsement by governmental authorities around the world. OPPT is an active participant in these meetings and accepts these documents as reliable screening-level hazard assessments.

These hazard characterizations are technical documents intended to inform subsequent decisions and actions by OPPT. Accordingly, the documents are not written with the goal of informing the general public. However, they do provide a vehicle for public access to a concise assessment of the raw technical data on HPV chemicals and provide information previously not readily available to the public.

³ U.S. EPA. Risk Assessment Guidelines; <http://cfpub.epa.gov/ncea/raf/rafguid.cfm>.

<p>Chemical Abstract Service Registry Number</p>	<p style="text-align: center;"><u>Sponsored Chemicals</u></p> <p style="text-align: center;">68784-38-3 30113-45-2 218141-16-3 151789-06-9 68479-04-9 151789-07-0</p> <p style="text-align: center;"><u>Supporting Chemicals</u></p> <p style="text-align: center;">28701-67-9 68511-40-0 112-18-5 112-69-6 112-90-3 124-28-7 61791-31-9</p>
<p>Chemical Abstract Index Name</p>	<p style="text-align: center;"><u>Sponsored Chemicals</u></p> <p style="text-align: center;">1-Propanamine, 3-(C8-10-alkyloxy) derivs. 1-Propanamine, 3-(isodecyloxy)- 1-Propanamine, 3-(C9-11-isoalkyloxy) derivs., C10-rich 1-Propanamine, 3-(C11-14-isoalkyloxy) derivs., C13-rich 1,3-Propanediamine, N-[3-(tridecyloxy)propyl]-, branched 1,3-Propanediamine, N-[3-(C11-14-isoalkyloxy)propyl] derivs., C13-rich</p> <p style="text-align: center;"><u>Supporting Chemicals</u></p> <p style="text-align: center;">1-Propanamine, 3-(isodecyloxy)-acetate 1-Propanamine, 3-(tridecyloxy)-, branched 1-Dodecanamine, N,N-dimethyl- 1-Hexadecanamine, N,N-dimethyl- 9-Octadecen-1-amine, (9Z)- 1-Octadecanamine, N,N-dimethyl- Ethanol, 2,2'-iminobis-, N-coco alkyl derivs.</p>
<p>Structural Formula</p>	<p style="text-align: center;">See Section 1</p>
<p style="text-align: center;">Summary</p> <p>Measured physical property data were not available for the sponsored chemicals of the Fatty Nitrogen-Derived (FND) Ether Amines category. Physical state data was also not provided. Based on data for the supporting chemicals, the substances in this category are likely to be oily liquids or</p>	

solids at room temperature. Vapor pressures are expected to range from low (for diamines CASRNs 68479-04-9 and 151789-07-0) to moderate (monoamines CASRNs 68784-38-3; 30113-45-2; 218141-16-3; 151789-06-9) based on estimated data for their representative structures. The monoamines of this category are expected to have high to moderate water solubility based on estimated data for their representative structures, and the diamines may be dispersible in water at neutral pH. The members of the FND Ether Amines category are expected to have low mobility in soil. Volatilization is not expected to be an important fate process for any category members since these substances are weak bases that will exist as cations in the environment, and cations do not volatilize. The rate of hydrolysis is expected to be negligible. The rate of atmospheric photooxidation is expected to be rapid for the members of this category; however, these substances are not expected to exist in the vapor phase. Given that supporting chemicals in this category were mostly readily biodegradable, members of the FND Ether Amines category are expected to be readily biodegradable. The members of the FND Ether Amines category are expected to have low persistence (P1). Bioaccumulation potential is expected to be low (B1) for the C10-rich mixtures (CASRNs 68784-38-3; 30113-45-2; and 218141-16-3) and moderate (B2) for the C13-rich mixtures (CASRNs 151789-06-9; 68479-04-9; and 151789-07-0).

Data on a single FND ether amines supporting chemical, CASRN 28701-67-9, indicates that the acute oral toxicity of the FND ether amines is low. The supporting chemical, CASRN 68511-40-0, was not mutagenic in bacteria *in vitro*. No adequate data were provided for the repeated-dose, reproductive, developmental toxicity and genetic toxicity (chromosomal aberrations) endpoints.

The 96-h LC₅₀ of CASRN 68479-04-9 for fish is 0.16 mg/L. The 30-day NOEC of the supporting chemical, 61791-31-9, for fish is 0.050 mg/L. The 48-h EC₅₀ of CASRN 68469-04-9 for aquatic invertebrates is 0.132 mg/L. The 96-h LC₅₀ of the supporting chemical, CASRN 112-90-3, for aquatic plants, is 0.03 mg/L.

The repeated-dose, reproductive, developmental toxicity and genetic toxicity (chromosomal aberrations) endpoints were identified as data gaps under the HPV Challenge Program.

The sponsor, the Nitrogen Derivatives Panel Amines Task Group of the American Chemistry Council, submitted a test plan and robust summaries to EPA for the Fatty Nitrogen-Derived (FND) Amines category on December 23, 2002. EPA posted the submission on the ChemRTK HPV Challenge website on January 23, 2003 (<http://www.epa.gov/oppt/chemrtk/pubs/summaries/amines/c14171tc.htm>). In a letter dated April 29, 2003, the sponsor indicated to EPA that a revision of the amines category would be submitted by December 31, 2003. In a letter dated July 10, 2003, the sponsor informed EPA of its plans to split the original submission into two separate submissions, an amines category and an ether amines category. A revised category containing the FND ether amines included in the original submission was submitted to EPA on December 29, 2003. EPA posted the submission on the ChemRTK HPV Challenge website on March 25, 2004. EPA comments on the revised FND ether amines category submission were posted to the website on October 26, 2007.

The hazard characterization for the FND amines category is being posted on the EPA website at the same time as this one because there is substantial overlap in the chemicals used in both categories. The original 2002 submission had 29 sponsored chemicals – the six in this submission plus 23 that were split off to form the FND amines category (all supporting information is available at the same URL used for this submission). Four of the six chemicals chosen for this hazard characterization (FND ether amines category) are sponsored or supporting chemicals in the FND amines category.

Category Justification

The FND ether amines category consists of six sponsored chemicals that include four long-chain substituted propanamines and two long-chain substituted propanediamines. The sponsor's rationale for grouping the six sponsored FND ether amines into a single category is based on the structural similarities of the chemicals (e.g., presence of ether and one or two amines) and similarities in their environmental fate and toxicity. The submitted data for the FND ether amines category appear consistent across the category for the physical and chemical properties, environmental fate and ecological effects and therefore, EPA agrees that the category is justified. No data were available for the sponsored substances for any human health endpoints. However, given similarities in chemical structure, EPA assumes that the metabolism and toxicity among these chemicals would be similar and agrees that these chemicals can be considered in the same category.

Justification for Supporting Chemicals

The sponsor proposed two FND ether amines and 22 FND amines as supporting chemicals.

For physical-chemical and environmental fate properties, several supporting chemicals are used. These include the chemicals used for the human health and aquatic toxicity endpoints and three additional chemicals (CASRN 112-18-5, 112-69-6 and 124-28-7) based on structural and physical-chemical properties to provide enough data with which to make a conclusion regarding biodegradation.

For human health endpoints, the two proposed FND ether amines (CASRN 28701-67-9 and 68511-40-0) are structurally similar to the category members and hence are reasonable supporting chemicals for the purposes of the HPV Challenge Program. However, the 22 FND amines were not used as supporting chemicals for human health endpoints for the following reasons: 1) the amines have no ether function and apparently no chain branching, which could result in differences in toxicities;

2) many of the non-ether amines have additional structural features that differ from the FND ether amines (e.g., multiple –OH groups); 3) no toxicity data are available for the category members to assess their similarities with the supporting chemicals; and 4) the test plan does not specifically describe how the supporting chemical data will be used to characterize the sponsored substances.

For aquatic toxicity endpoints, the data for the supporting chemical CASRN 112-90-3 was used to fill the aquatic plant toxicity endpoint based on similar physical and chemical properties, fate parameters, use of measured concentrations and because it was the most toxic of the supporting chemicals. In addition, CASRN 61791-31-9 was used because it was the only supporting chemical with chronic toxicity data.

1. Chemical Identity

1.1 Identification and Purity

The FND ether amines category consists of six substances. In addition, four non-sponsored chemicals are being used as support for this category. The structures of these compounds are presented in Table 1.

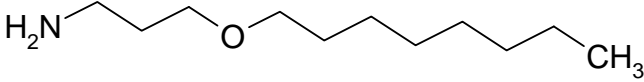
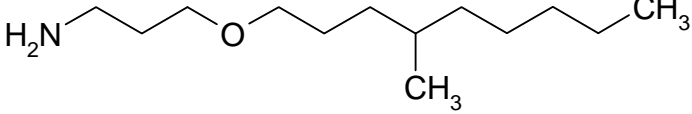
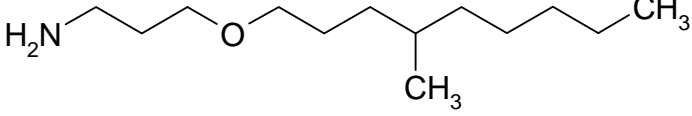
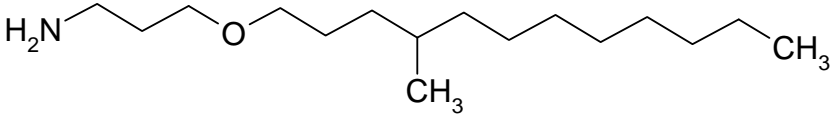
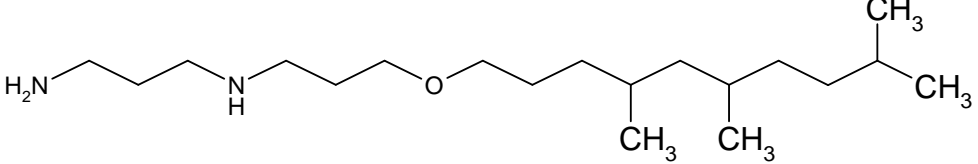
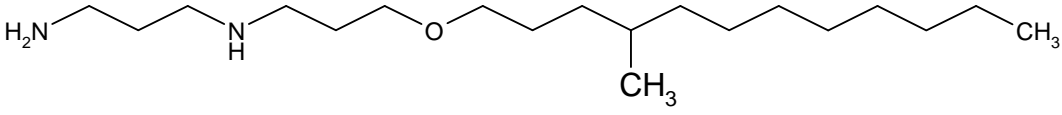
Table 1. Chemical Structures for FND Ether Amines Category		
Name	CASRN	Structure
Sponsored Chemicals		
1-Propanamine, 3-(C8-10-alkyloxy) derivs.	68784-38-3	 <p>Representative structure</p>
1-Propanamine, 3-(isodecyloxy)-	30113-45-2	 <p>Representative structure</p>
1-Propanamine, 3-(C9-11-isoalkyloxy) derivs., C10-rich	218141-16-3	 <p>Representative structure</p>
1-Propanamine, 3-(C11-14-isoalkyloxy) derivs., C13-rich	151789-06-9	 <p>Representative structure</p>
1,3-Propanediamine, N1-[3-(tridecyloxy)propyl]-, branched]	68479-04-9	 <p>Representative structure</p>
1,3-Propanediamine, N-[3-(C11-14-isoalkyloxy)propyl] derivs., C13-rich	151789-07-0	 <p>Representative structure</p>

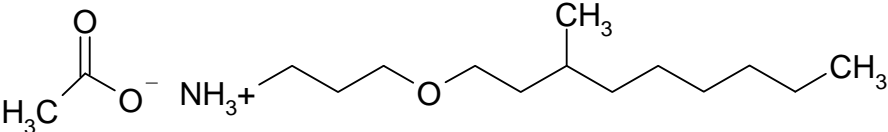
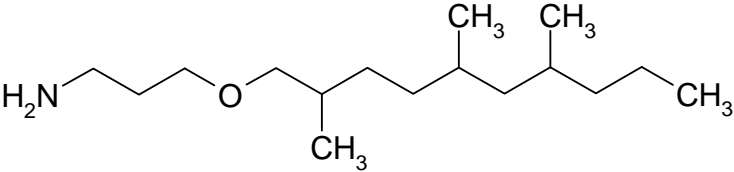
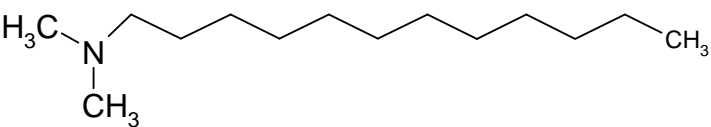
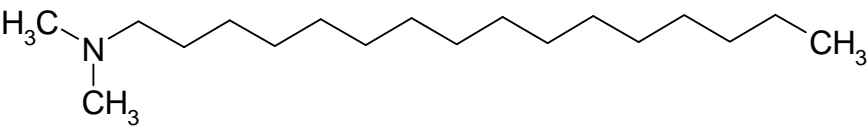
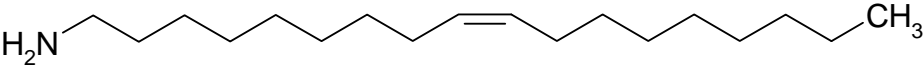
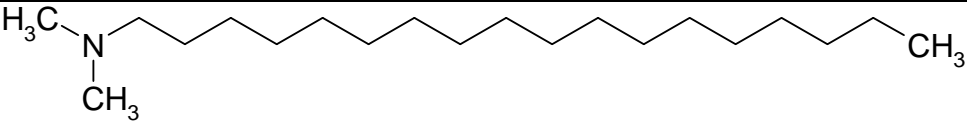
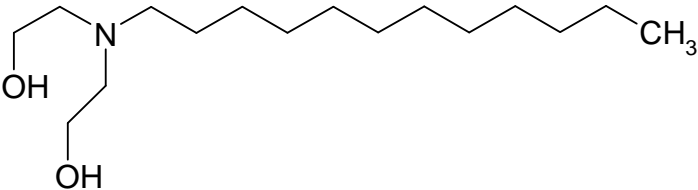
Table 1. Chemical Structures for FND Ether Amines Category		
Name	CASRN	Structure
Sponsored Chemicals		
1-Propanamine, 3-(isodecyloxy)-, acetate (1:1)	28701-67-9	
1-Propanamine, 3-(tridecyloxy)-, branched	68511-40-0	 Representative structure
1-Dodecanamine, N,N-dimethyl-	112-18-5	
1-Hexadecanamine, N,N-dimethyl-	112-69-6	
9-Octadecen-1-amine, (9Z)-	112-90-3	
1-Octadecanamine, N,N-dimethyl-	124-28-7	

Table 1. Chemical Structures for FND Ether Amines Category		
Name	CASRN	Structure
Sponsored Chemicals		
Ethanol, 2,2'-iminobis-, N-coco alkyl derivs.	61791-31-9	 <p style="text-align: right;">Representative structure¹</p>

¹ For coco (coconut) fatty amine mixtures, the sponsor provides the following distribution: 44–53% lauric amine; 13–19% myristic amine; 8–11% palmitic amine; 5–10% decanoic amine; 5–9% octanoic amine; 5–8% linoleic amine. The representative structures shown for coco fatty amines contain a saturated 12-carbon chain length, as it is the highest concentration in the mixture according to the sponsor.

The sponsor's December 29, 2003 test plan described features of the composition of the long chain groups of the sponsored and supporting category members. Only the features of the supporting chemicals that have been retained are described (see Table 2).

Table 2. Chain Length and Degree of Unsaturation for Long-Chain Substituents in the FND Ether Amines Category and Supporting Chemicals		
Identifier	Chain Length(s) or Average	Degree of Unsaturation
C8-C10 alkyl	9	None
Isodecyl	10	None
C9-C11 (C10 rich)	10	None
Dodecyl	12	None
Tridecyl	13	None
C11-C14 (C13 rich)	13	None
Hexadecyl	16	None
Octadecenyl	18	1
Coco (coconut)	C6: 0-1%	None
	C8: 5-9%	None
	C10: 5-10%	None
	C12: 44-53%	None
	C14: 13-19%	None
	C16: 8-11%	None
	C18: 1-3%	None
	C16: 0-1%	1
	C18: 5-8%	1
C18: 1-3%	2	

Source: p.4 of *Fatty Nitrogen Derived Ether Amines Category High Production Volume (HPV) Chemical Challenge* – test plan submitted on December 29, 2003.

1.2 Physical-Chemical Properties

The physical-chemical properties of the FND ether amines category are summarized in Tables 3 and 4.

Measured physical property data were not available for the sponsored chemicals of Fatty Nitrogen-derived (FND) Ether Amines. Physical state data for FND Ether Amines were not provided. Based on data for the supporting chemicals, the substances in this category are likely to be oily liquids or solids at room temperature. Vapor pressures are expected to range between low (for diamines CASRN 68479-04-9 and 151789-07-0) and moderate (monoamines CASRN 68784-38-3; 30113-45-2; 218141-16-3; 151789-06-9) based on estimated data for their representative structures. The monoamines of this category are expected to have high (CASRN 68784-38-3) to moderate water solubility based on estimated data for their representative structures. Estimated and measured vapor pressure and water solubility data for the supporting chemicals support these trends. The diamines may be dispersible at neutral pH. Therefore, discreet measurements or estimates of water solubility and log K_{ow} for these diamines may not be accurate.

Table 3. Physical-Chemical Properties of Fatty Nitrogen-Derived Ether Amines Category (Sponsored Chemicals)^{1,2}

Property	SPONSORED CHEMICAL 1-Propanamine, 3-(C8-10-alkyloxy) derivs.	SPONSORED CHEMICAL 1-Propanamine, 3-(isodecyloxy)-	SPONSORED CHEMICAL 1-Propanamine, 3-(C9-11-isoalkyloxy) derivs., C10-rich	SPONSORED CHEMICAL 1-Propanamine, 3-(C11-14-isoalkyloxy) derivs., C13-rich	SPONSORED CHEMICAL 1,3-Propanediamine, N1-[3-(tridecyloxy)propyl]-, branched]	SPONSORED CHEMICAL 1,3-Propanediamine, N-[3-(C11-14-isoalkyloxy)propyl] derivs., C13-rich
	Value	Value	Value	Value	Value	Value
CASRN	68784-38-3	30113-45-2	218141-16-3	151789-06-9	68479-04-9	151789-07-0
Molecular Weight	187 (typical)	215 (typical)	215 (typical)	257 (typical)	315 (typical)	315 (typical)
Physical State	No data	No data	No data	No data	No data	No data
Melting Point	No data	No data	No data	No data	No data	No data
Boiling Point	101°C at 1 mm Hg (measured) ³ 276°C (extrapolated) ^{3,4}	280°C (estimated) ⁵	280°C (estimated) ⁵	>300°C (estimated) ⁵	>300°C (estimated) ⁵	>300°C (estimated) ⁵
Vapor Pressure	4.5×10 ⁻³ mm Hg at 25°C (estimated) ⁴	3.5×10 ⁻³ mm Hg at 25°C (estimated) ⁵	3.5×10 ⁻³ mm Hg at 25°C (estimated) ⁵	1.7×10 ⁻⁴ mm Hg at 25°C (estimated) ⁵	7.0×10 ⁻⁶ mm Hg at 25°C (estimated) ⁵	2.2×10 ⁻⁶ mm Hg at 25°C (estimated) ⁵
Dissociation Constant (pK _a)	9.9 (estimated) ⁶	9.9 (estimated) ⁶	9.9 (estimated) ⁶	9.9 (estimated) ⁶	8.2–10 (estimated) ⁶	8.2–10 (estimated) ⁶
Henry's Law Constant	1.1×10 ⁻⁶ atm·m ³ /mole at 25°C (estimated) ⁵	2.0×10 ⁻⁶ atm·m ³ /mole at 25°C (estimated) ⁵	2.0×10 ⁻⁶ atm·m ³ /mole at 25°C (estimated) ⁵	4.7×10 ⁻⁶ atm·m ³ /mole at 25°C (estimated) ⁵	7.0×10 ⁻⁹ mm Hg at 25°C (estimated) ⁵	1.9×10 ⁻⁹ atm·m ³ /mole (estimated) ⁵
Water Solubility	1.4×10 ⁴ mg/L at 25°C (estimated) ⁵	170 mg/L (estimated) ⁵	170 mg/L at 25°C (estimated) ⁵	5.4 mg/L at 25°C (estimated) ⁵	Dispersible ⁷	Dispersible ⁷
Log K _{ow}	3.0 (estimated) ⁵	3.9 (estimated) ⁵	3.9 (estimated) ⁵	5.4 (estimated) ⁵	Not applicable ⁷	Not applicable ⁷

¹ American Chemistry Council. December 29, 2003. Revised Robust Summary and Test Plan for Fatty Nitrogen-Derived Ether Amines Category. Available online at <http://www.epa.gov/hpv/pubs/summaries/amines/c14171tc.htm>.

² Estimated data provided are based on the typical representative structure; see Table 1 for detailed information on the structures.

³ Beilstein Search. 2010.

⁴ NOMO5. 1987. Programs to Enhance PC-Gems Estimates of Physical Properties for Organic Compounds. The Mitre Corp.

⁵ U.S. EPA. 2010. Estimation Programs Interface Suite™ for Microsoft® Windows, v4.00. U.S. Environmental Protection Agency, Washington, DC, USA. Available online at <http://www.epa.gov/opptintr/exposure/pubs/episuitedl.htm> as of July 12, 2010.

⁶ SPARC On-Line Calculator. 2008. Version 4.2. Available online at <http://ibmlc2.chem.uga.edu/sparc> as of July 21, 2010.

⁷ Due to dispersibility, log K_{ow} cannot be reliably measured or estimated. Source: Tolls, J; Sijm, D. 2000. Estimating properties of surface active chemicals. In: Handbook of Property Estimation for Chemicals. Boethling, RS; Mackay, D; eds. Chapter 17. Lewis Publishers: Boca Raton, FL. pp. 419–446.

Table 4. Physical-Chemical Properties of Fatty Nitrogen-derived Ether Amines Category (Supporting Chemicals)^{1,2}							
Property	SUPPORTING CHEMICAL 1-Propanamine, 3-(isodecyloxy)-, acetate (1:1)	SUPPORTING CHEMICAL 1-Propanamine, 3-(tridecyloxy)-, branched	SUPPORTING CHEMICAL 1-Dodecanamine, N,N-dimethyl-	SUPPORTING CHEMICAL 1-Hexadecanamine, N,N-dimethyl-	SUPPORTING CHEMICAL 9-Octadecen-1-amine, (9Z)-	SUPPORTING CHEMICAL 1-Octadecanamine, N,N-dimethyl-	SUPPORTING CHEMICAL Ethanol, 2,2'-iminobis-, N-cocoalkyl derivs.
	Value	Value	Value	Value	Value	Value	Value
CASRN	28701-67-9	68511-40-0	112-18-5	112-69-6	112-90-3	124-28-7	61791-31-9
Molecular Weight	275.4	257 (typical)	213	270	267	298	273 (typical)
Physical State	No data	No data	Liquid ³	Liquid ³	Liquid ³	Liquid ³	Liquid ³
Melting Point	No data	No data	-15°C (measured) ³	8°C (measured) ³ ; 12°C (measured) ⁴	21°C (measured)	22.9°C (measured)	18.7–20.9°C (measured) ⁴
Boiling Point	>300°C (estimated) ⁶	>300°C (estimated) ⁶	260°C (measured) ⁹	147°C at 2 mm Hg (measured) ⁴ ; 319°C (extrapolated) ⁵	335°C (measured)	205–208°C at 16 mm Hg (measured) ⁴ ; 332–335°C (extrapolated) ⁵	179–183°C at 2 mm Hg (measured) ⁴ ; 358–363°C (extrapolated) ⁵
Vapor Pressure	<1×10 ⁻¹⁰ mm Hg at 25°C (estimated) ⁶	6.7×10 ⁻⁴ mm Hg at 25°C (estimated) ⁶	0.022 mm Hg (estimated) ⁵	3.3×10 ⁻⁴ mm Hg (estimated) ⁵	2.7×10 ⁻⁴ mm Hg (estimated) ⁵	1.4×10 ⁻⁴ mm Hg (estimated) ⁵	2.3×10 ⁻⁵ mm Hg (estimated) ⁵
Dissociation Constant (pK _a)	Not applicable	9.9 (estimated) ⁷	7.5 (estimated) ⁷	7.1 (estimated) ⁷	10.4 (estimated) ⁷	7.5 (estimated) ⁷	6.2 (estimated) ⁷
Henry's Law Constant	<1×10 ⁻¹⁰ atm-m ³ /mole at 25°C (estimated) ⁶	4.7×10 ⁻⁶ atm-m ³ /mole at 25°C (estimated) ⁶	8.2×10 ⁻⁴ atm-m ³ /mol (estimated) ⁶	2.6×10 ⁻³ atm-m ³ /mol (estimated) ⁶	8.2×10 ⁻⁴ atm-m ³ /mol (estimated) ⁶	4.5×10 ⁻³ atm-m ³ /mol (estimated) ⁶	1.9×10 ⁻⁹ atm-m ³ /mol (estimated) ⁶
Water Solubility	Dispersible ⁸	7.18 mg/L at 25°C (estimated) ⁶	9.3 mg/L (estimated) ⁶	0.10 mg/L (estimated) ¹⁰	0.08 mg/L (estimated) ⁶	0.44 mg/L (measured) ¹¹	Dispersible ⁸

Table 4. Physical-Chemical Properties of Fatty Nitrogen-derived Ether Amines Category (Supporting Chemicals)^{1,2}							
Property	SUPPORTING CHEMICAL 1-Propanamine, 3-(isodecyloxy)-, acetate (1:1)	SUPPORTING CHEMICAL 1-Propanamine, 3-(tridecyloxy)-, branched	SUPPORTING CHEMICAL 1-Dodecanamine, N,N-dimethyl-	SUPPORTING CHEMICAL 1-Hexadecanamine, N,N-dimethyl-	SUPPORTING CHEMICAL 9-Octadecen-1-amine, (9Z)-	SUPPORTING CHEMICAL 1-Octadecanamine, N,N-dimethyl-	SUPPORTING CHEMICAL Ethanol, 2,2'-iminobis-, N-cocoalkyl derivs.
	Value	Value	Value	Value	Value	Value	Value
Log K _{ow}	Not applicable ⁸	5.3 (estimated) ⁶	5.4 (estimated) ⁶	7.4 (estimated) ¹⁰	7.5 (estimated) ⁶	8.4 (estimated) ⁶	Not applicable ⁸

¹ American Chemistry Council. December 29, 2003. Revised Robust Summary and Test Plan for Fatty Nitrogen-Derived Ether Amines Category. Available online at <http://www.epa.gov/hpv/pubs/summaries/amines/c14171tc.htm>.

² Estimated data provided are based on the typical representative structure; see Table 1 for detailed information on the structures.

³ Visek, K. 2003. Amines, Fatty. Kirk-Othmer Encyclopedia of Chemical Technology. John Wiley & Sons, Inc. Article online posting date: August 15, 2003.

⁴ Beilstein Search. 2010.

⁵ NOMO5. 1987. Programs to Enhance PC-Gems Estimates of Physical Properties for Organic Compounds. The Mitre Corp.

⁶ U.S. EPA. 2010. Estimation Programs Interface Suite™ for Microsoft® Windows, v4.00. U.S. Environmental Protection Agency, Washington, DC, USA. Available online at <http://www.epa.gov/opptintr/exposure/pubs/episuitedi.htm> as of July 12, 2010.

⁷ SPARC Online Calculator. 2008. Version 4.2. Available online at <http://ibmlc2.chem.uga.edu/sparc/> as of July 21, 2010.

⁸ Due to dispersibility, log K_{ow} cannot be reliably measured or estimated. Source: Tolls, J; Sijm, D. 2000. Estimating properties of surface active chemicals. In: Handbook of Property Estimation for Chemicals. Boethling, RS; Mackay, D; eds. Chapter 17. Lewis Publishers: Boca Raton, FL. pp. 419–446.

⁹ SRC. 2010. The Physical Properties Database (PHYSPROP). SRC: Syracuse, NY. Available online at <http://www.srcinc.com/what-we-do/free-demos.aspx> as of July 16, 2010.

¹⁰ A measured water solubility value of 2 g/L provided by the sponsor was determined to be semi-quantitative and is not in good agreement with other measured data.

¹¹ Chemicals Inspection and Testing Institute. 1996. Biodegradation and Bioaccumulation Data of Existing Chemicals Based on the CSCL Japan. Japan Chemical Industry Ecology - Toxicology and Information Center. ISBN 4-89074-101-1, pg. 2–36.

1. General Information on Exposure

1.1 Production Volume and Use Pattern

The Ether Amines category chemicals had an aggregated production and/or import volume in the United States between 3 million pounds and 31 million pounds in calendar year 2005. The individual production ranges are as follows:

- CASRN 68784-38-3: < 500,000 pounds
- CASRN 218141-16-3: 1 to <10 million pounds
- CASRN 151789-06-9: 1 to <10 million pounds
- CASRN 68479-04-9: < 500,000 pounds
- CASRN 151789-07-0: 1 to <10 million pounds

CASRN 30113-45-2 was not reported under the 2006 Inventory Update Rule (IUR).

Non-confidential uses under the IUR are as follows:

CASRN 218141-16-3: Non-confidential information in the IUR indicated that the industrial processing and uses of the chemical include soap and cleaning compound manufacturing as intermediates; other basic organic chemical manufacturing and iron ore mining as functional fluids. Non-confidential commercial and consumer uses of this chemical include lubricants, greases and fuel additives.

CASRN 151789-06-9: Non-confidential information in the IUR indicated that the industrial processing and uses of the chemical include soap and cleaning compound manufacturing as intermediates; surface active agents. No commercial and consumer uses were reported for these chemicals.

CASRN 151789-07-0: Non-confidential information in the IUR indicated that the industrial processing and uses of the chemical include paint and coating manufacturing as adhesives and binding agents; soap and cleaning compound manufacturing as intermediates and surface active agents; iron ore mining and other metal ore mining as flotation agents. Non-confidential commercial and consumer uses of this chemical include paints and coatings.

CASRNs 68784-38-3 and 68479-04-9: No industrial processing and uses and commercial and consumer uses were reported for these chemicals.

2.2 Environmental Exposure and Fate

The environmental fate properties of the FND ether amines category are summarized in Tables 5 and 6. The members of the FND Ether Amines are expected to have low mobility in soil. Biodegradation data were available for several of the supporting chemicals in this category, with most studies indicating that FND amines are readily biodegradable according to OECD test guidelines or that they degrade

extensively. Volatilization of FND Ether Amines will be negligible since these substances are expected to exist as cations under environmental conditions, and ionic substances do not volatilize. Hydrolysis is expected to be negligible for these chemicals as they contain functional groups that do not hydrolyze or that hydrolyze slowly in the environment. If released to air, the rate of atmospheric photooxidation is expected to be rapid for all sponsored chemicals based on estimations for representative structures. FND Ether Amines are expected to have low persistence (P1). Bioaccumulation potential is expected to be low (B1) for the C10-rich mixtures (CASRN 68784-38-3; 30113-45-2; and 218141-16-3) and moderate (B2) for the C13-rich mixtures (CASRN 151789-06-9; 68479-04-9; and 151789-07-0).

Property	SPONSORED CHEMICAL 1-Propanamine, 3-(C8-10-alkoxy) derivs.	SPONSORED CHEMICAL 1-Propanamine, 3-(isodecyloxy)-	SPONSORED CHEMICAL 1-Propanamine, 3-(C9-11-isoalkoxy) derivs., C10-rich	SPONSORED CHEMICAL 1-Propanamine, 3-(C11-14-isoalkoxy) derivs., C13-rich	SPONSORED CHEMICAL 1,3-Propanediamine, N1-[3-(tridecyloxy)propyl]-, branched]	SPONSORED CHEMICAL 1,3-Propanediamine, N-[3-(C11-14-isoalkoxy)propyl] derivs., C13-rich
	Value	Value	Value	Value	Value	Value
CASRN	68784-38-3	30113-45-2	218141-16-3	151789-06-9	68479-04-9	151789-07-0
Photodegradation Half-life ³	2.1 hours (estimated)	2.0 hours (estimated)	2.0 hours (estimated)	1.9 hours (estimated)	0.8 hours (estimated)	0.8 hours (estimated)
Hydrolysis Half-life	Stable					
Biodegradation	No data	No data	No data	No data	No data	No data
Bioaccumulation Factor ³	BAF = 78 (estimated)	BAF = 320 (estimated)	BAF = 320 (estimated)	BAF = 1,296 (estimated)	BAF = 2,384 (estimated)	BAF = 3,228 (estimated)
Log K _{oc} ³	2.9 (estimated)	3.3 (estimated)	3.3 (estimated)	4.1 (estimated)	4.6 (estimated)	4.7 (estimated)
Fugacity (Level III Model) ³						
Air%	0.3	0.4	0.4	0.3	<0.1	<0.1
Water%	24.1	24.0	24.0	22.0	8.3	12.1
Soil%	74.9	74.0	74.0	69.4	73.5	70.4
Sediment%	0.6	1.6	1.6	8.2	18.2	17.5
Persistence ⁴	P1	P1	P1	P1	P1	P1
Bioaccumulation ⁴	B1	B1	B1	B2	B2	B2

¹ American Chemistry Council. December 29, 2003. Revised Robust Summary and Test Plan for Fatty Nitrogen-Derived Ether Amines Category. Available online at <http://www.epa.gov/hpv/pubs/summaries/amines/c14171tc.htm>.

² Estimated data provided are based on the representative structure (see Table 1).

³ U.S. EPA. 2010. Estimation Programs Interface Suite™ for Microsoft® Windows, v4.00. U.S. Environmental Protection Agency, Washington, DC, USA. Available online at <http://www.epa.gov/opptintr/exposure/pubs/episuitd.htm> as of July 12, 2010.

⁴ Federal Register. 1999. Category for Persistent, Bioaccumulative, and Toxic New Chemical Substances. *Federal Register* 64, Number 213 (November 4, 1999) pp. 60194–60204.

Table 6. Environmental Fate Characteristics of Fatty Nitrogen-Derived Ether Amines Category (Supporting Chemicals)^{1,2}							
Property	SUPPORTING CHEMICAL 1-Propanamine, 3-(isodecyloxy)-, acetate (1:1)	SUPPORTING CHEMICAL 1-Propanamine, 3-(tridecyloxy)-, branched	SUPPORTING CHEMICAL 1-Dodecanamine, N,N-dimethyl-	SUPPORTING CHEMICAL 1-Hexadecanamine, N,N-dimethyl-	SUPPORTING CHEMICAL 9-Octadecen-1-amine, (9Z)-	SUPPORTING CHEMICAL 1-Octadecanamine, N,N-dimethyl-	SUPPORTING CHEMICAL Ethanol, 2,2'-iminobis-, N-cocoalkyl derivs.
	Value	Value	Value	Value	Value	Value	Value
CASRN	28701-67-9	68511-40-0	112-18-5	112-69-6	112-90-3	124-28-7	61791-31-9
Photodegradation Half-life ³	2.6 hours (estimated)	1.8 hours (estimated)	1.4 hours (estimated)	1.3 hours (estimated)	1.2 hours (estimated)	1.3 hours (estimated)	1.1 hours (estimated)
Hydrolysis Half-life	Stable						
Biodegradation	No data	No data	67% in 28 days (readily biodegradable); 72% in 29 days (readily biodegradable)	59% in 28 days (readily biodegradable); >100% in 28 days (readily biodegradable)	66% in 28 days (not readily biodegradable) ⁵ ; >60% in 12 days (inherently biodegradable)	49% in 29 days (inherently biodegradable); 72% in 4 weeks (readily biodegradable) ⁶	61% in 28 days (readily biodegradable)
Bioaccumulation Factor ³	BAF = 6.2 (estimated)	BAF = 1,100 (estimated)	BAF = 280 (estimated)	BAF = 950 (estimated)	BAF = 2.1×10 ⁵ (estimated)	BAF = 1,400 (estimated)	BAF = 21 (estimated)
Log K _{oc} ³	2.4 (estimated)	4.0 (estimated)	3.8 (estimated)	4.8 (estimated)	5.3 (estimated)	5.3 (estimated)	2.2 (estimated)
Fugacity (Level III Model) ³	<0.1						
Air%	17.0	0.1	0.5	0.2	0.1	0.1	<0.1
Water%	83.0	15.7	16.8	10.7	13.9	14.6	22.1
Soil%	<0.1	75.2	79.8	72.5	57.8	71.9	77.7
Sediment%		9.0	2.9	16.7	28.2	13.3	0.2

Table 6. Environmental Fate Characteristics of Fatty Nitrogen-Derived Ether Amines Category (Supporting Chemicals)^{1,2}

Property	SUPPORTING CHEMICAL 1-Propanamine, 3-(isodecyloxy)-, acetate (1:1)	SUPPORTING CHEMICAL 1-Propanamine, 3-(tridecyloxy)-, branched	SUPPORTING CHEMICAL 1-Dodecanamine, N,N-dimethyl-	SUPPORTING CHEMICAL 1-Hexadecanamine, N,N-dimethyl-	SUPPORTING CHEMICAL 9-Octadecen-1-amine, (9Z)-	SUPPORTING CHEMICAL 1-Octadecanamine, N,N-dimethyl-	SUPPORTING CHEMICAL Ethanol, 2,2'-iminobis-, N-cocoalkyl derivs.
	Value	Value	Value	Value	Value	Value	Value
Persistence ⁴	P1 (low)	P1 (low)	P1 (low)	P1 (low)	P1 (low)	P1 (low)	P1 (low)
Bioaccumulation ⁴	B1 (low)	B2 (moderate)	B1 (low)	B1 (low)	B3 (high)	B2 (moderate)	B1 (low)

¹ American Chemistry Council. December 29, 2003. Revised Robust Summary and Test Plan for Fatty Nitrogen-Derived Ether Amines Category. Available online at <http://www.epa.gov/hpv/pubs/summaries/amines/c14171tc.htm>.

² Estimated data provided are based on the representative structure (see Table 1).

³ U.S. EPA. 2010. Estimation Programs Interface Suite™ for Microsoft® Windows, v4.00. U.S. Environmental Protection Agency, Washington, DC, USA. Available online from: <http://www.epa.gov/opptintr/exposure/pubs/episuitedi.htm> as of July 12, 2010.

⁴ Federal Register. 1999. Category for Persistent, Bioaccumulative, and Toxic New Chemical Substances. *Federal Register* 64, Number 213 (November 4, 1999) pp. 60194–60204.⁵ 60% biodegradation needs to be achieved within a 10-day window following the initial 10% degradation for the substance to be considered readily biodegradable.

⁶ National Institute of Technology and Evaluation. 2002. Biodegradation and Bioaccumulation of the Existing Chemical Substances under the Chemical Substances Control Law. Available online at http://www.safe.nite.go.jp/english/kizon/KIZON_start_hazkizon.html as of August 10, 2010.

3. Human Health Hazard

A summary of health effects data submitted for SIDS endpoints is provided in Table 7. The table also indicates where data for tested category members are read-across (RA) to untested members of the category.

Acute Oral Toxicity

1-Propanamine, 3-(isodecyloxy)-, acetate (CASRN 28701-67-9, supporting chemical)

HSD:SD rats (5/sex/dose) were administered CASRN 28701-67-9 via gavage at 1000, 1500 or 2000 mg/kg and observed for 14 days following dosing. Mortalities occurred at 1500 and 2000 mg/kg.

LD₅₀ = 1216 mg/kg

Repeated-Dose/Reproductive/Developmental Toxicity

No adequate data were provided for these endpoints.

Genetic Toxicity – Gene Mutations

1-Propanamine, 3-(tridecyloxy)-, branched (CASRN 68511-40-0, supporting chemical)

Salmonella typhimurium strains TA98, TA100, TA1535, TA1537 and TA1538 were exposed to CASRN 68511-40-0 in 100% ethanol at concentrations ranging from 0.33 to 100 µg/plate, with and without metabolic activation. These concentrations were chosen based on cytotoxicity observed at higher concentrations (up to 5000 µg/plate). Vehicle and positive controls were included although the responses of the control groups were not stated.

CASRN 68511-40-0 was not mutagenic in this assay.

Genetic Toxicity – Chromosomal Aberrations

No adequate data were provided for this endpoint.

Conclusions: Data on a single FND ether amines supporting chemical, CASRN 28701-67-9, indicates that the acute oral toxicity of the FND ether amines is low. The supporting chemical, CASRN 68511-40-0, was not mutagenic in bacteria *in vitro*. No adequate data were provided for the repeated-dose, reproductive, developmental toxicity and genetic toxicity (chromosomal aberrations) endpoints.

Table 7. Summary of the Screening Information Data Set – Human Health Data

Endpoints	SPONSORED CHEMICAL 1-Propanamine, 3-(C₈₋₁₀-alkyloxy) derivatives (68784-38-3)	SPONSORED CHEMICAL 1-Propanamine, 3-(C₁₁₋₁₄-isoalkyloxy) derivs., C₁₃ rich (151789-06-9)	SPONSORED CHEMICAL 1,3-Propanediamine, N-(3-(C₁₁₋₁₄-isoalkyloxy) propyl) derivs., C₁₃ rich (151789-07-0)	SPONSORED CHEMICAL 1-Propanamine, 3-(isodecyloxy)- (30113-45-2)	SPONSORED CHEMICAL 1-Propanamine, 3-(C₉₋₁₁-isoalkyloxy) derivs., C₁₀ rich (218141-16-3)	SPONSORED CHEMICAL 1,3-Propanediamine, N-[3-(tridecyl-oxy)propyl]-, branched (68479-04-9)	SUPPORTING CHEMICAL 1-Propanamine, 3-(isodecyloxy)-, acetate (28701-67-9)	SUPPORTING CHEMICAL 1-Propanamine, 3-(tridecyloxy)-, branched (68511-40-0)
Acute Oral Toxicity LD₅₀ (mg/kg)	No Data 1216 (RA)	No Data 1216 (RA)	No Data 1216 (RA)	No Data 1216 (RA)	No Data 1216 (RA)	No Data 1216 (RA)	1216	–
Repeated-Dose Toxicity NOAEL/LOAEL	No Data	No Data	No Data	No Data	No Data	No Data	–	–
Reproductive Toxicity NOAEL/LOAEL	No Data	No Data	No Data	No Data	No Data	No Data	–	–
Developmental Toxicity NOAEL/LOAEL	No Data	No Data	No Data	No Data	No Data	No Data	–	–
Genetic Toxicity – Gene Mutations	No Data Negative (RA)	No Data Negative (RA)	No Data Negative (RA)	No Data Negative (RA)	No Data Negative (RA)	No Data Negative (RA)	–	Negative
Genetic Toxicity – Chromosomal Aberrations	No Data	No Data	No Data	No Data	No Data	No Data	–	–

Measured data in bold text; (RA) = Read Across; – indicates that endpoint was not evaluated for this substance

4. Hazard to the Environment

A summary of aquatic toxicity data submitted for SIDS endpoints is provided in Table 8. The table also indicates where data for tested category members are read-across (RA) to untested members of the category.

Acute Toxicity to Fish

1,3-Propanediamine, N-[3-(tridecyloxy)propyl]-, branched (CASRN 68479-04-9)

Fathead minnows (*Pimephales promelas*) were exposed to CASRN 68479-04-9 at nominal concentrations of 0.04, 0.07, 0.15, 0.3, 0.6 and 1.0 mg/L under static-renewal conditions for 96 hours. Measured concentrations were not provided. Test details were not stated.

96-h LC₅₀ = 0.16 mg/L

cis-9-Octadecenylamine (CASRN 112-90-3, supporting chemical)

Fathead minnows (*Pimephales promelas*) were exposed to CASRN 112-90-3 at nominal concentrations of 0.05, 0.09, 0.15, 0.27 and 0.49 mg/L under static conditions for 96 hours. Measured concentrations were 0.032, 0.12, (0.27 mg/L nominal concentration not provided) and 0.40 mg/L. No mortality occurred at ≤ 0.09 mg/L; complete mortality occurred at ≥ 0.15 mg/L.

96-h LC₅₀ = 0.11 mg/L

Acute Toxicity to Aquatic Invertebrates

1,3-Propanediamine, N-[3-(tridecyloxy)propyl]-, branched (CASRN 68479-04-9)

Ceriodaphnia dubia were exposed to CASRN 68469-04-9 at nominal concentrations of 0.04, 0.07, 0.15, 0.3 and 0.6 mg/L under static-renewal conditions for 48 hours. Measured concentrations were not provided. Mortalities occurred at all dose levels.

48-h LC₅₀ = 0.132 mg/L

cis-9-Octadecenylamine (CASRN 112-90-3, supporting chemical)

Waterfleas (*Daphnia magna*) were exposed to CASRN 112-90-3 at nominal concentrations of 0.006, 0.11, 0.023, 0.045 and 0.090 mg/L under static conditions for 48 hours. Measured concentrations in the control, 0.011, 0.023 and 0.090 mg/L nominal solutions were 0.007, 0.013, 0.020 and 0.077 mg/L.

Immobilities occurred in the control and at ≥ 0.011 mg/L.

48-h EC₅₀ = 0.011 mg/L

Toxicity to Aquatic Plants

cis-9-Octadecenylamine (CASRN 112-90-3, supporting chemical)

Green algae (*Pseudokirchneriella subcapitata*) were exposed to CASRN 112-90-3 at nominal concentrations of 0.01, 0.02, 0.04, 0.08 or 0.15 mg/L under static conditions for 96 hours. Measured concentrations in control, 0.01, 0.04 and 0.15 mg/L were 0, not detected (ND), 0.016, 0.011 and ND mg/L. Test result details were not provided.

96-h EC₅₀ = 0.03 mg/L

Chronic Toxicity to Fish

Ethanol, 2,2'-iminobis-, N-coco alkyl derivatives (CASRN 61791-31-9, supporting chemical)

Zebra fish (*Brachydanio rerio*) were exposed to CASRN 61791-31-9 at measured concentrations of 0.027, 0.049, 0.050, 0.11 and 0.15 mg/L under flow-through conditions for 28 days. Larvae survival was the only indicator of an effect of this test substance on the fathead minnow. Survival of larvae at 0.11 and 0.15 mg/L was less than controls.

30-d LC₅₀ = 0.0179 mg/L

30-d NOEC = 0.050 mg/L

Conclusion: The 96-h LC₅₀ of CASRN 68479-04-9 for fish is 0.16 mg/L. The 30-day NOEC of the supporting chemical, 61791-31-9, for fish is 0.050 mg/L. The 48-h EC₅₀ of CASRN 68469-04-9 for aquatic invertebrates is 0.132 mg/L. The 96-h LC₅₀ of the supporting chemical, CASRN 112-90-3, for aquatic plants, is 0.03 mg/L.

Table 7. Summary of the Screening Information Data Set as Submitted under the U.S. HPV Challenge Program – Aquatic Toxicity Data (Ether Amine Chemicals)

Endpoints	SPONSORED CHEMICAL 1-Propanamine, 3-(C₈₋₁₀-alkyloxy) derivatives (68784-38-3)	SPONSORED CHEMICAL 1-Propanamine, 3- (C₁₁₋₁₄-isoalkyloxy) derivs., C₁₃ rich (151789-06-9)	SPONSORED CHEMICAL 1,3- Propanediamine, N-(3-(C₁₁₋₁₄-isoalkyloxy) propyl) derivs., C₁₃ rich (151789-07-0)	SPONSORED CHEMICAL 1-Propanamine, 3-(isodecyloxy)- (30113-45-2)	SPONSORED CHEMICAL 1-Propanamine, 3- (C₉₋₁₁-isoalkyloxy) derivs., C₁₀ rich (218141-16-3)	SPONSORED CHEMICAL 1,3- Propanediamine, N-[3-(tridecyl- oxy)propyl]-, branched (68479-04-9)	SUPPORTING CHEMICAL cis-9-Octa- decylamine (112-90-3)	SUPPORTING CHEMICAL N-coco alkyl derivatives of 2,2'- iminobis ethanol (61791-31-9)
Fish 96-h LC₅₀ (mg/L)	No Data 0.16 (RA)	No Data 0.16 (RA)	No Data 0.16 (RA)	No Data 0.16 (RA)	No Data 0.16 (RA)	0.16 (m)	-	-
Aquatic Invertebrates 48-h EC₅₀ (mg/L)	No Data 0.132 (RA)	No Data 0.132 (RA)	No Data 0.132 (RA)	No Data 0.132 (RA)	No Data 0.132 (RA)	0.132 (m)	-	-
Aquatic Plants 92-h EC₅₀ (mg/L)	No Data 0.03 (RA)	No Data 0.03 (RA)	No Data 0.03 (RA)	No Data 0.03 (RA)	No Data 0.03 (RA)	No Data 0.03 (RA)	0.03 (m)	-
Chronic Toxicity to Fish 30-day NOEC (mg/L)	No Data 0.050 (RA)	No Data 0.050 (RA)	No Data 0.050 (RA)	No Data 0.050 (RA)	No Data 0.050 (RA)	No Data 0.050 (RA)	-	0.050 (m)

(m) = measured data (i.e., derived from testing); (RA) = Read Across; - indicates that endpoint was not evaluated for this substance