Alkyldimethylbenzylammonuim Chloride (ADBAC) Category High Production Volume (HPV) Chemicals Challenge Final Test Status and Data Review

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Final Test Status

ADBAC Category		Information	Guideline Study	GLP	Other Study	Estimation Method	Acceptable	Testing Required
STUDY		**Y/N**	**Y/N**	**Y/N**	**Y/N**	**Y/N**	**Y/N**	**Y/N**
PHYSICAL AND CHEMICAL DATA								
2.1	Melting Point	Y	Y	Y	N	N	Y	N
2.2	Boiling Point	Y	N	N	N	N	Y	N
2.4	Vapour Pressure	Y	Y	Y	Y	N	Y	N
2.5	Partition Coefficient	Y	N	N	N	Y	Y	N
2.6	Water Solubility	Y	Y	Y	N	N	Y	N
ENVIRONMENTAL FATE AND PATHWAY								
3.1.1	Photodegradation	Y	Y	Y	N	N	Y	N
3.1.2	Stability in Water	Y	Y	Y	N	N	Y	N
3.3	Transport and Distribution	Y	Y	Y	N	N	Y	N
3.5	Biodegradation	Y	Y	Y	N	N	Y	N
ECOTOXICITY								
4.1	Acute Toxicity to Fish	Y	Y	Y	N	N	Y	N
4.2	Toxicity to Daphnia	Y	Y	Y	N	N	Y	N
4.3	Toxicity to Aquatic Plants, e.g. Algae	Y	Y	Y	N	N	Y	N
4.5	Chronic Toxicity	Y	Y	Y	N	N	Y	N
TOXICITY								
5.1	Acute Toxicity	Y	N	N	Y	N	Y	N
5.4	Repeated Dose Toxicity	Y	Y	Y	N	N	Y	N
5.5	Genotoxicity *In Vitro* (Bacterial Test)	Y	Y	Y	N	N	Y	N
5.5	Genotoxicity *In Vitro* (Mammalian Cells)	Y	Y	Y	N	N	Y	N
5.6	Genotoxicity *In Vivo*	Y	Y	Y	N	N	Y	N
5.8	Reproductive Toxicity	Y	Y	Y	N	N	Y	N
5.9	Development Toxicity / Teratogenicity	Y	Y	Y	N	N	Y	N

ADBAC Category
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1.0 Introduction

Surfactants have a long history of safe use and have been studied extensively for environmental fate and effects and human health effects. The ADBAC (Alkyl Dimethyl Benzyl Ammonium Chlorides) Category chemicals are similar to other cationic surfactants with respect to physical/chemical properties, environmental fate and toxicity. The chemicals included in the ADBAC Category are FIFRA registered antimicrobial chemicals with germicidal, fungicidal and algicidal activity. They are used extensively as bactericides, fungicides, sanitizers, deodorants and disinfectants in the restaurant, dairy, food, laundry and medical industries (Henderson, 1992).

2.0 Definition of ADBAC Structure-Based Chemical Category

The ADBAC Category is comprised of three separate quaternary ammonium compounds (quats) with unique Chemical Abstracts Service Registry Numbers (CAS RNs; see Text Table A).

The U. S. EPA clustered quaternary ammonium compounds into four groups for the purpose of toxicology testing needed for reregistration under FIFRA (U. S. EPA, 1988). Based on their structures, the ADBAC Category chemicals all fit into EPA Group II of the EPA clustering scheme. EPA designated alkyl (C12-16) dimethylbenzyl ammonium chloride (ADBAC; CAS RN 68424-85-1) as the representative member of Group II, meaning that data developed for this chemical would be representative for the other quats in Group II. For the purpose of determining environmental toxicity, ADBAC (C12-16) remained the representative member of the group (U.S. EPA, 1993). It was determined during the testing for reregistration under FIFRA that the quats included in EPA Group II all had similar toxicological, environmental fate and ecotoxicological profiles. Since the ADBAC Category chemicals appropriately fit into the EPA scheme, the data for ADBAC [Alkyl (C12-16) dimethylbenzyl ammonium chloride] adequately fulfill the data needs for all three chemicals in the ADBAC Category defined in Text Table A.

The ADBAC Category chemicals are identified in the following table:

Text Table A: CAS Registry Numbers and Chemical Names

CAS RN	Chemical Name
68424-85-1 (ADBAC)	Alkyl (C12-16) dimethylbenzyl ammonium chloride (ADBAC C12-16)
68391-01-5	Alkyl (C12-18) dimethylbenzyl ammonium chloride (ADBAC C12-18)
122-19-0	Benzyldimethyloctadecyl ammonium chloride

3.0 General Substance Information (Identity)

The following table presents the molecular formula and molecular weight data for the chemicals with defined structures or structures for which average chain lengths can be determined. The structures for these and the remaining chemicals in the ADBAC Category are provided in Table 1.

Text Table B: Molecular Formula and Molecular Weight of Chemicals with Defined Structures

CAS RN	Chemical Name	Molecular Formula	Molecular Weight
68424-85-1 (ADBAC)	Alkyl (C12-16) dimethylbenzyl ammonium chloride (ADBAC C12-16)	$C_9 H_{13} N Cl^- R$ $R = C_{12} H_{25}$, $C_{14} H_{29}$ or $C_{16} H_{33}$	359.6 [a]
68391-01-5	Alkyl (C12-18) dimethylbenzyl ammonium chloride (ADBAC C12-18)	$C_9 H_{13} N Cl^- R$ $R = C_{12} H_{25}$, $C_{14} H_{29}$, $C_{16} H_{33}$ or $C_{18} H_{37}$	377.8 [b]
122-19-0	Benzyldimethyloctadecyl ammonium chloride	$C_{27}H_{50}NCl$	424.2

[a] Based on chain length distribution of the most frequently tested ADBAC C12-16: C12 (40%), C14 (50%), C16 (10%).

[b] Based on most representative chain length distribution of ADBAC C12-18: C12 (57%), C14 (18%), C16 (7%), C18 (18%).

4.0 Rationale for the ADBAC Structure-Based Chemical Category

The ADBAC Category surfactants are included as a single HPV chemical category based on the following similarities:

- Chemical structural and functional similarities of cationic surfactants;
- Similar measured or modeled physical properties such as melting point, boiling point, vapor pressure, partition coefficient (log K_{ow}) and water solubility;
- Similar biodegradability;
- Aquatic toxicity observed at low concentrations consistent with cationic surfactants in general;
- Minimal mammalian toxicity;
- Similar uses and release patterns in the environment;
- Chemicals of the ADBAC Category fit into a "clustering" group (Group II) established by EPA during the reregistration of quaternary ammonium compounds used as antimicrobials under FIFRA.

5.0 General Use and Exposure

The production of Alkyldimethylbenzyl ammonium chloride is carried out by fully trained personnel, wearing appropriate personal protective clothing. The appropriate environmental controls are in place to ensure that environmental and personal exposure is negligible.

ADBAC is a general disinfectant that kills microorganisms by direct contact and destruction of cell walls. Therefore, it is used against a broad spectrum of organisms including many bacteria and viruses. ADBAC is also an effective algaecide and has selective activity against fungi.

6.0 Available Data to Fulfill HPV Screening Information Data Set (SIDS) Endpoints

6.1 Availability of Reliable Data for the ADBAC Category

Robust Summaries for SIDS/HPV endpoint studies and other supporting studies with reliable data (according to Klimisch *et al.*, 1997) for the ADBAC Category chemicals are provided in Appendix A and are summarized in Tables 2 through 4.

Reliable data were available for physical and chemical properties as shown in the following table:

Text Table C: Number of Available Reliable Physical/Chemical Properties Studies

CAS RN	Melting Point (°C)	Boiling Point (°C)	Vapor Pressure (hPa)	Partition Coefficient (log K_{ow})	Water Solubility (g/L)
68424-85-1 (ADBAC)	**1**		**1**		**1**
68391-01-5			**1**		**1**
122-19-0					

Note: Empty block denotes data either are not available or are available and judged inadequate.

Reliable data were available for photodegradation, biodegradation and aquatic toxicity endpoints as shown in the following table:

Text Table D: Number of Available Reliable Environmental Fate and Ecotoxicity Studies

CAS RN	Photo-degradation	Stability in Water	Transport and Distribution	Bio-degradation	Acute Toxicity to Fish	Acute Toxicity to Invertebrates	Other
68424-85-1 (ADBAC)	**1**	**1**	**2**	**2**	**6**	**4**	**4**
68391-01-5				**2**			
122-19-0				**2**			

Note: Empty block denotes data either are not available or are available and judged inadequate.

Reliable data were available for human health-related toxicity endpoints as shown in the following table:

Text Table E: Number of Available Reliable Human Health-Related Studies

CAS RN	Acute Oral Tox.	Acute Dermal Tox.	Repeated Dose Tox.	*In vitro* Genetic Tox.	Tox. to Reproduction	Develop-mental Tox.	Other
68424-85-1 (ADBAC)	**1**	**1**	**7**	**4**	**1**	**2**	**1**
68391-01-5	**1**	**1**				**1**	
122-19-0						**1**	

Note: Empty block denotes data either are not available or are available and judged inadequate.

6.2 Physical/Chemical Properties QSAR Estimates and Correlation to Reliable Data

The physical/chemical property estimation program EPIWIN v.4.00 (U.S. EPA, 2009) was used to derive estimates for applicable endpoints. The estimates are based on structure and, therefore, can be made only for substances for which a structure can be defined. The QSAR estimates for physical/chemical properties of the ADBAC Category chemicals are presented in Table 2.

Experimental physical/chemical properties data were available for two ADBAC Category chemicals (ADBAC C12-16 and ADBAC C12-18), and a complete set of model data was generated for one of the three ADBAC Category chemicals with a discrete structure (benzyldimethyloctadecyl ammonium chloride; CAS RN 122-19-0). The compositional diversity of the two chemicals without definable structures made the experimental measurement of

physical/chemical properties of these chemicals of minimal practical value for prediction of their environmental behavior or toxicological properties. Therefore, the other chemicals in the Category for which the properties can be measured and/or modeled best support the chemicals in the ADBAC Category without defined structures.

The available data for physical/chemical properties are summarized below:

For the two chemicals with experimental data (ADBAC C12-16 and ADBAC C12-18), melting point and boiling point could not be defined due to the fact that decomposition began at approximately 150°C. As such, these measurements were technically unfeasible. For benzyldimethyloctadecyl ammonium chloride (CAS RN 122-19-0), EPIWIN predicted melting and boiling points of 263 and 607°C, respectively; however, the estimated values should be interpreted with caution considering the temperature at which ADBAC C12-16 and ADBAC C12-18 begin to decompose.

Both the experimental and EPIWIN estimated vapor pressures were very low. The ADBAC Category chemicals are essentially nonvolatile, as is generally the case for long chain length organic molecules of this size and complexity.

For the ADBAC Category chemicals, the surface active properties and high solubility in octanol and water do not allow for experimental determination of the log K_{ow}. An EPIWIN estimate for benzyldimethyloctadecyl ammonium chloride (CAS RN 122-19-0) revealed a log K_{ow} value of 5.87; however, this should be interpreted with caution due the limitations of the database. The software database is very limited for surface active materials since experimental values cannot be readily measured as discussed above. Experimental values for ADBAC C12-16 and ADBAC C12-18 revealed high water solubility (> 350 g/L). For benzyldimethyloctadecyl ammonium chloride (CAS RN 122-19-0), model predictions for water solubility showed that it was poorly soluble (0.02 mg/L).

Summary – Physical/Chemical Properties

For the ADBAC Category, melting and boiling points cannot be determined as decomposition begins without a clear melting or boiling point. Both experimental and estimated vapor pressure values are very low; the ADBAC Category chemicals are considered to be essentially nonvolatile. Log K_{ow} values could not be determined for the two lowest molecular weight chemicals (ADBAC C12-16 and ADBAC C12-18), and the modeled log K_{ow} for benzyldimethyloctadecyl ammonium chloride (CAS RN 122-19-0) was approximately 6.0. Water solubility estimates and measurements varied from poorly soluble to very soluble. As noted previously, measurement and prediction of physical/chemical properties for surfactants are complicated by their behavior in test systems and the environment, and the K_{ow} is not an appropriate hydrophobicity parameter for reliably predicting environmental behavior. Although predictions vary, the overall data and knowledge of the chemicals support the conclusion that the ADBAC Category chemicals with closely-related structures behave similarly from the perspective of physical/chemical properties.

6.3 Environmental Fate and Ecotoxicity QSAR Estimates and Correlation to Reliable Data

The available reliable data and QSAR estimates for the environmental fate and effects of the ADBAC Category chemicals are presented in Table 3. Robust Summaries for the reliable studies are provided in Appendix A.

A measurement of the photodegradation of ADBAC C12-16 in aqueous solution indicated that ADBAC C12-16 is photolytically stable in water. However, in the presence of a photosensitizer, acetone, the half life was calculated to be 10.9 days (83% degradation after 30 days), and essentially all of the ^{14}C-moiety not present as parent compound was found in one degradate. Models of atmospheric photodegradation predicted half-lives of approximately 2.6-2.8 hours for ADBAC C12-18 and benzyldimethyloctadecyl ammonium chloride (CAS RN 122-19-0).

The HYDROWIN model did not provide estimates of stability in water for this class of chemicals because the model cannot calculate this parameter for chemicals that do not meet the criteria of neutral organic compounds with structures that can be hydrolyzed. However, a measurement of stability in water showed that ADBAC C12-16 is hydrolytically stable under the conditions of the test (i.e., pH range 5-9, 25ºC).

An estimation of the transport and distribution of the ADBAC Category chemicals in environmental media (percent in air, water, soil and sediment) following entry into the environment via water (1000 kg/hr) is presented in Table 3. For ADBAC C12-16, the closely related C12-C18 compound, and benzyldimethyloctadecyl ammonium chloride (CAS RN 122-19-0), the model predicted the majority of distribution to sediment (> 95%) with the remainder primarily in water. Additionally, measured data were available for ADBAC C12-16 and indicated that ADBAC C12-16 is immobile in four soil/sediment types (average K_{oc} = 2.66E06) and rapidly dissipates from the water layer to the sediment layer (DT_{50} was 0.3 days for TNO and Kromme Rijn systems) and remains in sediment until degraded (whole system DT_{50} was >120 and 32 days for TNO and Kromme Rijn systems, respectively).

Because of the toxicity of the ADBAC Category chemicals to microorganisms, their biodegradation can be affected depending on test conditions. Measured data exist for all three of the ADBAC Category chemicals for the biodegradation endpoint. Since the ADBAC Category chemicals are thought to be released primarily into wastewater treatment systems (Boethling and Lynch, 1992), removal from these systems is an important measure of potential for environmental impact. The soluble organic carbon (SOC) of ADBAC C12-16 was approximately 100% removed in a simulated treatment process. For the closely related ADBAC C12-C18 compound, 72% of the test substance had degraded after 28 days, meeting the 10-day window, and 5% degraded at a higher concentration, showing toxicity to organisms. In another study with ADBAC C12-18, 95.5% degraded after 28 days. Both studies were conducted with activated sludge. Results of two biodegradation studies for benzyldimethyloctadecyl ammonium chloride (CAS RN 122-19-0) indicated little degradation or almost complete degradation depending on chemical and/or bacterial concentrations. Modeled values are of limited use due to the toxicity of the ADBAC Category chemicals to microorganisms.

Acute Effects

Experimental data on acute exposure were available for ADBAC C12-16. Measured acute fish toxicity data were available (LC_{50} values of 0.28 mg/L to 1.4 mg/L) for ADBAC C12-16. ADBAC C12-16 was tested on three freshwater species under semi-static conditions. Lethal effects were observed for the most sensitive species (Fathead minnow) with an LC_{50} value of 0.28 mg/L, measured. The LC_{50} value for a marine fish species tested (Sheepshead minnow was 0.86 mg/L. Modeled data for ADBAC C12-18 and benzyldimethyloctadecyl ammonium chloride (CAS RN 122-19-0), revealed estimated 96-hr LC_{50} values of 0.52 and 0.13 mg/L, respectively, for fish.

For algae exposed to ADBAC C12-16, the NOE_rC was not specified in the original study as the effects on growth rate occurred at higher concentrations than the effects on biomass and the NOE_bC (0.0012 mg/L) represented the lowest NOEC for both endpoints. In a study conducted to evaluate toxicity to the marine diatom, *Skeletonema costatum*, the 96-hour NOEC for cell density, biomass, and growth rate was 0.035 mg/L. The EC_{50} value for biomass (the most sensitive endpoint) was 0.058 mg/L. The aquatic plant, *Lemna gibba* was not affected by ADBAC C12-16 at 0.019 mg/L measured (NOAEC growth). Modeled data for ADBAC C12-18 and benzyldimethyloctadecyl ammonium chloride (CAS RN 122-19-0), revealed estimated 96-hr EC_{50} values of 0.87 and 0.32 mg/L, respectively, for algae.

The aquatic invertebrate, *Daphnia magna* was sensitive to ADBAC C12-16 with a 48-hr EC_{50} of 0.0058 mg/L. ADBAC also exhibited acute toxicity to the mysid (*Mysidopsis bahia*) and the Eastern oyster (*Crassostrea virginica*) in static saltwater systems with a 96-hr LC_{50} value of 0.092 mg/L and a 48-hr EC_{50} value of 0.048 mg/L, respectively. Modeled data for ADBAC C12-18 and benzyldimethyloctadecyl ammonium chloride (CAS RN 122-19-0), revealed estimated 48-hr LC_{50} values of 0.47 and 0.13 mg/L, respectively, for *D. magna*.

Long-Term Effects

The long-term toxicity of ADBAC C12-16 has been assessed for fish, invertebrates and sediment dwelling organisms. The compound showed no effects on the reproduction and growth of the fish species, Fathead minnow, at a concentration of 32.2 µg/L. No effect on the reproduction of *Daphnia magna* and *Mysidopsis bahia* were observed at concentrations of 4.15 µg/L and 8.0 µg/L, respectively. When tested in a water-sediment system under static conditions, no effects on the survival/growth of *Chironomus tentans* were observed at concentrations of 260 mg/kg dw.

Summary – Environmental Fate and Ecotoxicity

ADBAC C12-16 is hydrolytically and photolytically stable in water (i.e., in the absence of a photosensitizing agent). Fugacity modeling for distribution of the ADBAC Category chemicals in the environment indicated that sediment was the primary compartment for distribution (> 95%), with the remainder primarily in water and limited or no distribution to soil or air. Biodegradation studies indicate that the ADBAC Category chemicals are removed adequately from treatment plants and, under appropriate conditions and concentrations, are inherently to readily biodegradable. Additionally, cationic substances in the environment spontaneously form

complexes with naturally occurring negatively charged constituents in sewage, soils, sediments and with dissolved humic substances in surface waters. This complexation behavior results in reduced bioavailability in actual environmental conditions that is not adequately represented by standard laboratory assays and/or predictions by EPIWIN models. The available data support the conclusion that, because of their closely related structures, ADBAC Category chemicals possess similar environmental fate and ecotoxicity properties across the category.

The results of acute and long-term ecotoxicity studies indicate that ADBAC C12-16 is toxic to fish and invertebrates and algae. Aquatic plants are also affected in acute studies. The most sensitive group is invertebrates (*Daphnia*), and the least sensitive group is aquatic plants (*Lemna*). The toxicity of ADBAC Category chemicals to sediment dwelling organisms is low.

6.4 Human Health-Related Reliable Data

The human health-related data for SIDS endpoints of the three ADBAC Category chemicals are presented in Table 4. Robust Summaries for the reliable studies are provided in Appendix A.

Rat acute oral toxicity LD_{50} values of 0.43 ml/kg (approximately 344 mg/kg) and 850 mg/kg were established for ADBAC C12-16 and ADBAC C12-18, respectively. Acute dermal LD_{50} values of 3.56 ml/kg (approximately 2848 mg/kg) and 2300 mg/kg were established for ADBAC C12-16 and ADBAC C12-18, respectively. An extensive number of repeated dose oral toxicity studies, including subchronic and chronic studies in rats and mice were available for ADBAC C12-16. At high doses (approximately 500 mg/kg/day), ADBAC C12-16 was lethal to rats and mice due to localized effects in the gastrointestinal tract. At doses below those that result in severe, direct effects on the gastrointestinal (g.i.) tract, these repeated-dose oral toxicity studies revealed no organ-specific toxicity. Responses in 90-day and chronic toxicity studies were limited to body weight changes and other general responses. The NOAELs from subchronic and chronic studies across species ranged from approximately 14 mg/kg/day in a chronic dog study to approximately 192 mg/kg/day in a subchronic mouse study.

ADBAC C12-16 produced no mutagenic activity in any screening studies including *in vitro* (bacterial or mammalian cell mutation, mammalian cell chromosomal aberration and DNA synthesis) and *in vivo* (erythrocyte micronucleus) studies. The available data indicate that the chemicals in the ADBAC Category are unlikely to be mutagenic, as would be expected based on the structures, molecular weights and knowledge of related chemicals.

A two-generation reproduction study in rats was available for ADBAC C12-16. The NOAEL for toxicity was approximately 73 mg/kg/day for parents and offspring with no reproductive effects noted.

Developmental toxicity studies were available for ADBAC C12-16, ADBAC C12-18, and benzyldimethyloctadecyl ammonium chloride (CAS RN 122-19-0). For ADBAC C12-16, the oral maternal and developmental NOAELs were 10 and > 100 mg/kg/day, respectively, for rats, and 3 and > 9 mg/kg/day for rabbits, with no embryo/fetal toxicity or teratogenicity observed. For ADBAC C12-18, the oral maternal and developmental NOAELs were 15 and > 50 mg/kg/day, respectively, for rats. For benzyldimethyloctadecyl ammonium chloride (CAS RN 122-19-0), no maternal toxicity (other than local irritation), no developmental toxicity, and no

embryo/fetal toxicity or teratogenicity were observed following a maximum dose of 0.5 ml/day of a 6.6% solution (approximately 33 mg of test material per day).

Summary – Human Health-Related Data

The oral and dermal LD_{50} values indicate slight to moderate acute toxicity of the ADBAC Category chemicals. Repeated dose toxicity studies supported the conclusion that the chemicals in the ADBAC Category have minimal toxicity potential at doses below acutely toxic doses, which cause direct effects to the gastrointestinal tract. Available *in vitro* and *in vivo* assays indicated that the ADBAC Category chemicals are unlikely to have mutagenic activity. A two-generation reproductive toxicity study, and results from available developmental toxicity studies showed that the ADBAC Category chemicals are not reproductive or developmental toxicants. The available data and the EPA's inclusion of these chemicals as a "clustering" group for the reregistration of quaternary ammonium compounds used as antimicrobials under FIFRA support the conclusion that, because of their closely-related structures and similar surfactant properties, ADBAC Category chemicals possess similar human health-related data across the category.

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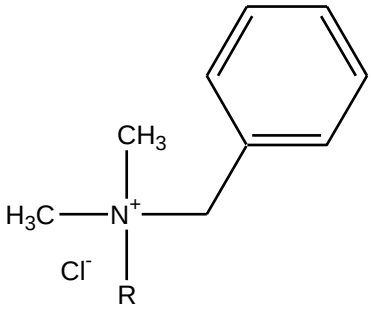
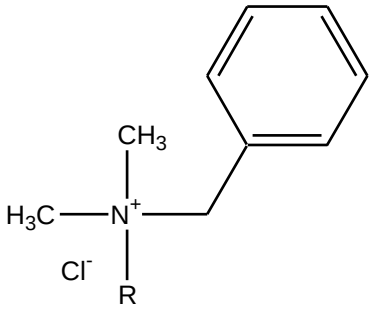
Table 1

Structures of ADBAC Category Chemicals



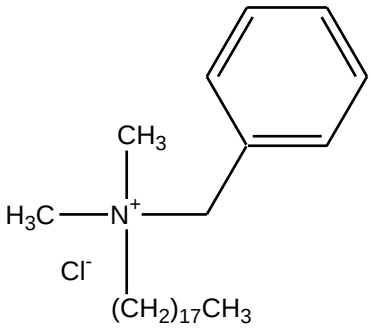
R = C_{12} – C_{16} alkyl

Alkyl (C12-16) dimethylbenzyl ammonium chloride
68424-85-1 (ADBAC)



R = C_{12} – C_{18} alkyl

Alkyl (C12-18) dimethylbenzyl ammonium chloride
68391-01-5



Benzyldimethyloctadecyl ammonium chloride
122-19-0

Table 2

Physical/Chemical Properties Data for ADBAC Category Chemicals

CAS RN	Melting Point (°C)	Boiling Point (°C)	Vapor Pressure (hPa)	Partition Coefficient (log K_{ow})	Water Solubility (g/L)
68424-85-1	Not performed; technically not feasible[a] *(Fischer 2001a)*	Not performed; technically not feasible[a] *(Fischer 2001a)*	6.03E-06, 8.57E-06 and 4.22E-05 hPa at 20, 25 and 50°C, respectively (*Franke 2001)*	Not determined; technically not feasible[b]	pH5.5: 409 g/L pH 6.5: 431 g/L pH 6.9: 403 g/L pH 8.2: 379 g/L All measurements performed at 20°C *(Fischer 2001b)*
68391-01-5	Not performed; technically not feasible[a] *(Fischer 2001a)*	Not performed; technically not feasible[a] *(Fischer 2001a)*	6.0E-06 hPa at 25ºC; 4.0E-06 hPa at 20ºC (*Sydney 2009)*	Not determined; technically not feasible[b]	500 - 1000 g/L at pH 5, 7 and 9 at room temperature (*Sydney 2009)*
122-19-0	263 (estimated)[c]	607 (estimated) [c]	1.59E-13 (estimated) [c]	5.87[b] (estimated) [c]	2.0E-5 (estimated) [c]

[a] The test substance does not possess a melting or boiling point; decomposition begins at approximately 150°C
[b] Assessment by KOWWIN was deemed inaccurate because the software database is very limited for surfactants.
[c] Estimated (EPIWIN, U.S. EPA, 2009)
NC = Not calculable

Table 3

Environmental Fate and Ecotoxicity Data for ADBAC Category Chemicals

CAS RN	Photodegradation	Stability in Water	Transport & Distribution	Biodegradation	Acute Toxicity to Fish	Acute Toxicity to Aquatic Invertebrates	Toxicity to Aquatic Plants	Additional Studies
68424-85-1	Direct photolysis: 0% after 30 days; $t_{1/2}$ = ≥30 days Indirect photolysis: (acetone): 83% degradation after 30 days; $t_{1/2}$ = 10.9 days (*Carpenter and Fennessey 1988a*)	Hydrolytically stable (pH 5-9, 25ºC) (*Carpenter and Fennessey 1988b*)	Immobile in four soil/sediment types (Average K_{oc} = 2.66E06) . *(Daly and Cranor 1988)* Rapidly dissipates from the water layer to the sediment layer in water/sediment systems (DT_{50} = >120 days, TNO; DT_{50} = 32 days, Kromme Rijn system) *(De Vette et al. 2001)* Air: <0.1% Water: 2.8% Soil: <0.1% Sediment: 97.2% (estimated)[a]	100% SOC removal [b] *(Corby 1992a)* Readily biodegradable: > 80% TCO_2 at 28 days[c] *(Corby 1992b; Van Dievoet and Bouillon 2005)*	96-Hr LC_{50} : Bluegill sun fish: 0.515 mg/L *(Pate and McIntyre 1991a)* Fathead minnow: 0.28 mg/L in dilution water *(Sword and Stuerman 1994a)* 0.77 or 1.4 mg/L in dilution water with 10 or 20 mg/L humic acid, respectively *(Sword and Stuerman 1994b; Sword and Stuerman 1994c)* Rainbow trout: 0.93 mg/L *(Pate and McIntyre 1991b)* Sheepshead minnow: 0.86 mg/L *(Sved et al. 1992a)*	*Daphnia magna* 48-Hr : EC_{50} = 0.0058 mg/L NOEC = <0.006 mg/L *(Pate and McIntyre 1991c)* 48-Hr : EC_{50} = 0.016 mg a.s./L NOEC = 0.012 mg a.s./L *(Jenkins 2007)* Eastern Oyster 48-Hr: EC_{50} = 0.048 mg/L LC_{50} = 0.055 mg/L NOEC = 0.025 mg/L *(Sved et al. 1992b)* Saltwater mysid 96-Hr: LC_{50} = 0.092 mg/L NOEC = 0.047 mg/L *(Sved et al. 1992c)*	*Selenastrum capricornutum* 72-Hr: NOE_bC: 0.0012 mg/L E_bC_{50}[1]: 0.014 mg/L E_rC_{50}[2]: 0.049 mg/L *(Mayer et al. 2001)* *Skeletonema costatum* 96-Hr: NOE_rC: 0.035 mg/L E_bC_{50}[1]: 0.058 mg/L E_rC_{50}[2]: 0.089 mg/L *(Desjardins et al. 2005a)* *Lemna gibba* 7-Day: EC_{50}: 0.12 mg a.s./L E_bC_{50}: 0.13mg a.s./L E_rC_{50}: Frond Number: 0.25 mg a.s./L Biomass: 0.37 mg a.s./L NOAEC (growth) = 0.019 mg a.s./L NOAEC (biomass; growth rates) = 0.043 mg a.s./L *(Desjardins et al. 2005b)*	**Chronic toxicity - Fish (Fathead minnow)** LC_{50} = 94 µg/L LOEC (hatchability) = 488.7 µg/L NOEC (hatchability) = 273.2 µg/L NOEC (survival) =32.2 µg/L NOEC (growth) >32.2 µg/L *(McIntyre and Pate 1992a)* **Chronic toxicity – Daphnia:** **NOEC** and LOEC **≥ 4.15 µg/L** NOEC (reproduction) = 4.15 µg/L LOEC (reproduction) = 5.02 µg/L NOEC + LOEC (growth) ≥ 4.15 µg/L MATC = 4.56 µg/L *(McIntyre and Pate 1992b)*

Table 3 (continued)

Environmental Fate and Ecotoxicity Data for ADBAC Category Chemicals

CAS RN	Photodegradation (cm^3/molecule-sec)	Stability in Water	Transport & Distribution	Biodegradation	Acute Toxicity to Fish	Acute Toxicity to Aquatic Invertebrates	Toxicity to Aquatic Plants	Additional Studies
68424-85-1 (continued)								**Chronic toxicity – Midge:** NOEC = 520 mg/kg LOEC = 1200 mg/kg LC_{50} = 479 mg/kg MATC = 790 mg/kg NOEC (growth) = 520 mg/kg LOEC (growth) = 1200 mg/kg *(England and Leak 1995)* **Chronic toxicity – Mysid:** NOEC = 8.0 µg/L LOEC = 16 µg/L *(Blankinship et al. 2006)*

Table 3 (continued)

Environmental Fate and Ecotoxicity Data for ADBAC Category Chemicals

CAS RN	Photodegradation	Stability in Water	Transport & Distribution	Biodegradation	Acute Toxicity to Aquatic Fish	Acute Toxicity to Aquatic Invertebrates	Toxicity to Aquatic Plants	Additional Studies
68391-01-5	Overall OH Rate Constant = 4.6 E-11 $t_{1/2}$ = 0.233 days (12-hr day; 1.5E6 OH/cm^3)	NC	Air: <0.1% Water: 2.14% Soil: <0.1% Sediment: 97.9% (estimated)[a]	Readily Biodegradable; activated sludge, 28 days: 72% (5 mg/L as DOC) 5% (10 mg/L as DOC) *(Bazzon and Deschamps 2002)* Readily Biodegradable; activated sludge, 28 days: 95.5% (5 mg carbon/L) *(Van Dievoet and Bouillon 2005)*	0.52 mg/L (96-hr LC_{50}) (estimated)[a]	0.47 mg/L (48-hr LC_{50}) (estimated)[a]	0.87 mg/L (96-hr EC_{50}) (estimated)[a]	
122-19-0	4.9E-12 $t_{1/2}$ = 0.217 days (12-hr day; 1.5E6 OH/cm^3)	NC	Air: <0.1% Water: 2.62% Soil: <0.1% Sediment: 97.4% (estimated)[a]	0% degraded in 10 d (*Van Ginkel 1995*) 94% degraded (SCAS)[b] (*Boethling et al. 1997*)	0.13 mg/L (96-hr LC_{50}) (estimated)[a]	0.13 mg/L (48-hr LC_{50}) (estimated)[a]	0.32 mg/L (96-hr EC_{50}) (estimated)[a]	

[a] Estimated (EPIWIN, U.S. EPA, 2009); based C16 alkyl chain length of ADBAC C12-16 and C18 alkyl chain length of ADBAC C12-18.
[b] Removal of soluble organic carbon (SOC) in a semi-continuous activate sludge (SCAS) removal test
Note: Empty block denotes data are either not available or are available and judged inadequate.
NC = Not calculable.

Table 4

Human Health-Related Data for ADBAC Category Chemicals

CAS RN	Acute Oral Toxicity LD_{50}	Acute Dermal Toxicity LD_{50}	Repeated Dose Toxicity NOAEL (mg/kg/day)	Genetic Toxicity *In vitro*	Toxicity to Reproduction NOAEL (mg/kg/day)	Developmental Toxicity/Teratogenicity NOAEL (mg/kg/day)	Additional Studies
68424-85-1	0.43 ml/kg (~ 344 mg a.s./kg) *(Wallace 1975)*	3.56 ml/kg (~ 2848 mg a.s./kg) *(Levenstein 1977)*	192[a] *(Van Miller and Weaver 1988a)* 70 [b] *(Van Miller and Weaver 1988b)* 20 [c] *(Gill and Wagner 1990)* 31 [d] *(Goldenthal 1994a)* 14 [e] *(Goldenthal 1994b)* 82 [f] *(Gill et al. 1991a)* 50 [g] *(Gill et al. 1991b)*	Negative (Ames) *(Thompson 2001)* Negative (Chromosomal Aberration) *(Durward 2001)* Negative (HGPRT) *(Young 1989)* Negative (UDS) *(Cifone 1989; McKeon 1992)*	Parents/ Offspring ≈ 73 Reproduction ≥ 145 *(Neeper-Bradley 1990)*	Maternal = 10 Developmental > 100 [h] *(Neeper-Bradley 1992)* Maternal = 3 Developmental > 9 [i] *(Neeper-Bradley and Kubena 1992)*	Negative (*in vivo* micronucleus) *(Kallesen 1985)*
68391-01-5	850 mg/kg *(Bailey 1976)*	2300 mg/kg *(Palanker 1976)*				Maternal = 15 Developmental > 50[h] *(Knickerbocker & Stevens 1977)*	
122-19-0						Maternal/ Developmental = 6.6% (approximately 33 mg/d) [j] No developmental toxicity was observed. *(Palmer et al. 1983)*	

[a] 13-Week feeding study in mice
[b] 13-Week feeding study in rats
[c] 13-Week dermal study in rats
[d] 8-Week dietary dose range-finding study in dogs
[e] 1-Year dietary study in dogs
[f] 78-Week dietary oncogenicity study in mice; adequate for SIDS/HPV reproductive screening; NOAEL based on toxicity - no carcinogenicity observed.
[g] Combined 2-year chronic dietary toxicity/oncogenicity study in rats; NOAEL based on toxicity - no carcinogenicity observed.
[h] Developmental toxicity/teratogenicity study in rats via oral gavage
[i] Developmental toxicity/teratogenicity study in rabbits via oral gavage
[j] Developmental toxicity/teratogenicity study in rats via dermal application
Note: Empty block denotes data either are not available or are available and judged inadequate.