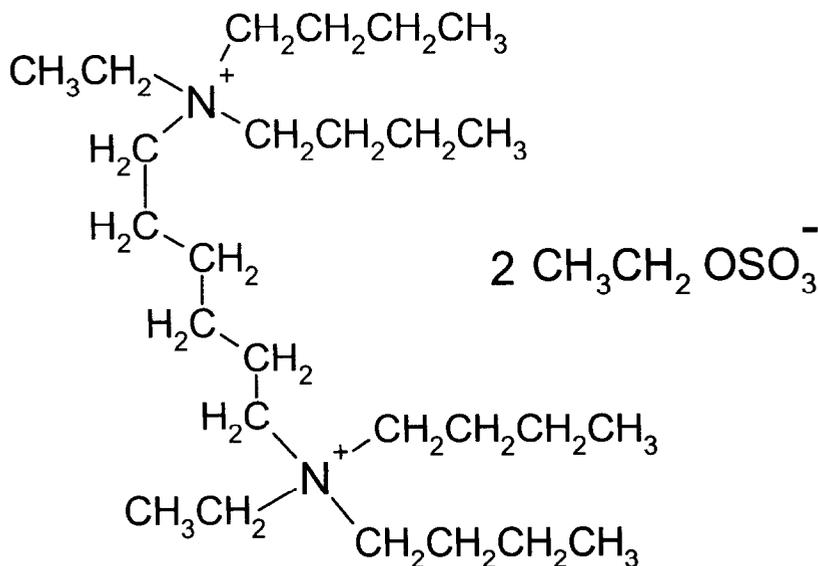


HPV Data Set



04 JAN 13 PM 12:42

RECEIVED
OPPT/CRIC

BQAES

Existing Chemical	: ID: 68052-49-3
CAS No.	: 68052-49-3
EINECS Name	: S,S'-diethyl N,N'-hexane-1,6-diylbis(dibutylethylammonium) disulphate
EC No.	: 268-327-3
Molecular Formula	: C ₂₆ H ₅₈ N ₂ .2C ₂ H ₅ O ₄ S
Producer related part	
Company	: Solutia Inc
Creation date	: 02.01.2005
Substance related part	
Company	: Toxicology and Regulatory Affairs
Creation date	: 02.01.2005
Status	: Prepared by: Toxicology and Regulatory Affairs Freiburg IL 62243 rauckman@toxicsolutions.com
Memo	: BQAES
Printing date	: 09.01.2005
Revision date	:
Date of last update	: 04.01.2005
Number of pages	: 17

1.0.1 APPLICANT AND COMPANY INFORMATION

Type : manufacturer
Name : Soluita Inc
Contact person :
Date :
Street :
Town :
Country :
Phone :
Telefax :
Telex :
Cedex :
Email :
Homepage :

04.01.2005

1.2 SYNONYMS AND TRADENAMES

2.1 MELTING POINT

Value : <= 318 °C
 Sublimation :
 Method : other: Calculated
 Year :
 GLP :
 Test substance : other TS

Method :

This material is produced, handled and disposed of as an aqueous solution containing up to 48% organic content. The melting point for the solid material has not been recorded as it is not isolated, but as an impure salt it is expected to be relatively high and variable. For the purpose of an HPV program, the melting point of the solid was estimated with the MPBPWIN (v 1.4) program. This estimate is considered an upper limit of the practical melting point for the solid. Due to limitations of the estimation software the cation and anion (as the sodium salt) portions of the molecule was separately estimated.

Result :

MPBPWIN (v1.40) Program Results:

=====

CATION

Experimental Database Structure Match: no data

SMILES : CCCCN(CCCC)(CC)CCCCCN(CCCC)(CCCC)(CC)

CHEM : BQAOH++ (twice charged form)

MOL FOR: C26 H58 N2

MOL WT : 398.77

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	6	-CH3	-5.10	-30.60
Group	20	-CH2-	11.27	225.40
Group	2	>N< (+5)	340.00	680.00
*		Equation Constant		122.50
RESULT		MELTING POINT in deg Kelvin		997.30
RESULT-limit		MELTING POINT in deg Kelvin		623.00
		MELTING POINT in deg C		349.84

Melting Point: 349.84 deg C (Adapted Joback Method)

Melting Point: 309.98 deg C (Gold and Ogle Method)

Mean Melt Pt : 329.91 deg C (Joback; Gold,Ogle Methods)

Selected MP: 317.95 deg C (Weighted Value)

2. Physico-Chemical Data

Id 68052-49-3

Date 09.01.2005

ANION

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	1	-CH3	-5.10	-5.10
Group	1	-CH2-	11.27	11.27
Group	2	-O- (nonring)	22.23	44.46
Group	1	>S(=O)(=O)	150.00	150.00
Group	1	Metal (Na,K,Li)	350.00	350.00
*		Equation Constant		122.50

RESULT	MELTING POINT in deg Kelvin	673.13
RESULT-limit	MELTING POINT in deg Kelvin	623.00
	MELTING POINT in deg C	349.84

Melting Point: 349.84 deg C (Adapted Joback Method)

Melting Point: 162.22 deg C (Gold and Ogle Method)

Mean Melt Pt : 256.03 deg C (Joback; Gold,Ogle Methods)

Selected MP: 199.75 deg C (Weighted Value)

- Test substance** : Solid portion of aqueous solution, BQAES CASNO 688052-49-3
- Conclusion** : The actual melting point of the solid portion of this material is expected to vary, depending on the impurity level, with a maximum of 318 °C
- Reliability** : (2) valid with restrictions
- Estimates calculated by a reliable method are assigned a reliability score of 2 (reliable with restrictions).
- Flag** : Critical study for SIDS endpoint
02.01.2005 (4)
- Value** : ca. -6.4 °C
- Sublimation** :
- Method** : other: Calculated for solution
- Year** :
- GLP** :
- Test substance** : as prescribed by 1.1 - 1.4
- Method** :
- The material as produced is an aqueous solution containing up to 48% BQAOH. The practical freezing point of the solution is a function of the solvent's freezing point and the freezing point depression caused by the solute. An approximate freezing point can be calculated based on the molal freezing-point depression constant for water of 1.86°C
- Result** :
- For a 48% solution of BQAES in water the approximate molality is 1.1. Considering that there could be up to three ions, the freezing point depression could be as great as 6.4°C.
- Conclusion** :
- The freezing point range for this material as an aqueous solution is 0 to -6.4°C; however, limits on the solubility could cause precipitated solid formation prior to freezing.
- Reliability** : (2) valid with restrictions

Estimates calculated by a reliable method are assigned a reliability score of 2 (reliable with restrictions).

Flag : Critical study for SIDS endpoint
02.01.2005 (1)

2.2 BOILING POINT

Value : ca. 100 - 102 °C at
Decomposition :
Method : other: Calculated for solution
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4

Method :
The material as produced is an aqueous solution containing up to 48% BQAES. The practical boiling point of the solution is a function of the solvent's boiling point and the boiling point elevation caused by the solute. An approximate boiling point can be calculated based on the molal boiling-point elevation constant for water of 0.52°C/m.

Remark :
The solid material is expected to decompose before boiling as it is a high molecular weight salt.

Result :
For a 48% solution of BQAOH in water, the approximate molality is 01.11. Considering that there could be up to three ions, the boiling-point elevation could be as great as 1.8°C.

Conclusion :
The initial boiling point range for this material as an aqueous solution is 100 to 102°C.

Reliability : (2) valid with restrictions
Estimates calculated by a reliable method are assigned a reliability score of 2 (reliable with restrictions).

Flag : Critical study for SIDS endpoint
02.01.2005 (1)

2.3 DENSITY

2.4 VAPOUR PRESSURE

Value : < .00000001 hPa at 25 °C
Decomposition :
Method : other (calculated)
Year :
GLP :
Test substance : other TS

2. Physico-Chemical Data

Id 68052-49-3
Date 09.01.2005

Method

The vapor pressure for a charged salt is expected to be negligible. In addition, as this material is produced and handled as an aqueous solution, the Henry's law constant is a more important factor for exposure consideration from bulk material or material that is introduced into the water column. EPIWIN was used to provide estimates for both the vapor pressure and the Henry's law constant. Due to limitations of the estimation software the cation and anion (as the sodium salt) portions of the molecule was separately estimated.

Result

:

CATION

MPBPWIN (v1.40) Program Results:

Experimental Database Structure Match: no data

SMILES : CCCC(CCCC)(CC)CCCCCN(CCCC)(CCCC)(CC)
CHEM : BQAOH++ (twice charged form)
MOL FOR: C26 H58 N2
MOL WT : 398.77

----- SUMMARY MPBPWIN v1.40 -----
Vapor Pressure Estimations (25 deg C):
(Using BP: 725.54 deg C (estimated))
(Using MP: 317.95 deg C (estimated))
VP: 8.95E-026 mm Hg (Antoine Method)
VP: 1.73E-017 mm Hg (Modified Grain Method)
VP: 8.8E-017 mm Hg (Mackay Method)
Selected VP: 1.73E-017 mm Hg (Modified Grain Method)

HENRY (v3.10) Program Results:

Bond Est : 5.15E-014 atm-m3/mole
Group Est: Incomplete

SMILES : CCCC(CCCC)(CC)CCCCCN(CCCC)(CCCC)(CC)
CHEM : BQAOH++ (twice charged form)
MOL FOR: C26 H58 N2
MOL WT : 398.77

----- HENRYWIN v3.10 Results -----

CLASS	BOND CONTRIBUTION	DESCRIPTION	COMMENT	VALUE
HYDROGEN	58	Hydrogen to Carbon (aliphatic) Bonds		-6.9413
FRAGMENT	19	C-C		2.2098
FRAGMENT	8	C-N		10.4080
FACTOR	*	Quaternary ammonium-type cmpd	ESTIMATE	6.0000
RESULT		BOND ESTIMATION METHOD for LWAPC VALUE	TOTAL	11.676

HENRY'S LAW CONSTANT at 25 deg C = 5.15E-014 atm-m3/mole
= 2.11E-012 unitless

Henry's LC [VP/WSol estimate using EPI values]:

HLC: 3.796E-021 atm-m3/mole
VP: 1.73E-017 mm Hg
WS: 2.39E+003 mg/L

ANION

MPBPWIN (v1.40) Program Results:

Experimental Database Structure Match: no data

2. Physico-Chemical Data

Id 68052-49-3

Date 09.01.2005

SMILES : CCOS(=O)(=O)O[Na]
CHEM : Sodium monoethylsulfate
MOL FOR: C2 H5 O4 S1 Na1
MOL WT : 148.11

----- SUMMARY MPBPWIN v1.40 -----

Boiling Point: 472.48 deg C (Adapted Stein and Brown Method)

Melting Point: 349.84 deg C (Adapted Joback Method)

Melting Point: 162.22 deg C (Gold and Ogle Method)

Mean Melt Pt : 256.03 deg C (Joback; Gold,Ogle Methods)

Selected MP: 199.75 deg C (Weighted Value)

Vapor Pressure Estimations (25 deg C):

(Using BP: 472.48 deg C (estimated))

(Using MP: 199.75 deg C (estimated))

VP: 7.11E-011 mm Hg (Antoine Method)

VP: 1.94E-009 mm Hg (Modified Grain Method)

VP: 5.33E-009 mm Hg (Mackay Method)

Selected VP: 1.94E-009 mm Hg (Modified Grain Method)

HENRY (v3.10) Program Results:

=====

Bond Est : 1.08E-008 atm-m3/mole

Group Est: Incomplete

SMILES : CCOS(=O)(=O)O[Na]
CHEM : Sodium monoethylsulfate
MOL FOR: C2 H5 O4 S1 Na1
MOL WT : 148.11

----- HENRYWIN v3.10 Results -----

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	5 Hydrogen to Carbon (aliphatic) Bonds		-0.5984
FRAGMENT	1 C-C		0.1163
FRAGMENT	1 C-O		1.0855
FRAGMENT	2 O-S	ESTIMATE	0.4200
FRAGMENT	2 O=S (sulfone-type)	ESTIMATE	2.1000
FRAGMENT	1 O-Na	ESTIMATE	3.2300
RESULT	BOND ESTIMATION METHOD for LWAPC VALUE	TOTAL	6.353

HENRYs LAW CONSTANT at 25 deg C = 1.08E-008 atm-m3/mole
= 4.43E-007 unitless

	GROUP CONTRIBUTION DESCRIPTION	COMMENT	VALUE
	1 CH3 (X)		-0.62
	1 CH2 (C)(O)		-0.13
	MISSING Value for: O (S)(C)		
	MISSING Value for: S (=O)(=O)(O)(O)		
	MISSING Value for: O (Na)(S)		
	MISSING Value for: UNTYPED(O)		
RESULT	GROUP ESTIMATION METHOD for LOG GAMMA VALUE	INCOMPLETE	-0.75

Henrys LC [VP/WSol estimate using EPI values]:

HLC: 3.781E-016 atm-m3/mole

VP: 1.94E-009 mm Hg

WS: 1E+006 mg/L

2. Physico-Chemical Data

Id 68052-49-3
Date 09.01.2005

Test substance : BQAES CASNO 68052-49-3

Conclusion : The estimated vapor pressure is negligible at 2.2E-17 hPa for the cation and 2.6E-9 hPa for the anion.

Reliability : (2) valid with restrictions
Estimates calculated by a reliable method are assigned a reliability score of 2 (reliable with restrictions).

Flag : Critical study for SIDS endpoint
02.01.2005 (3)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : at °C
pH value :
Method : other (calculated)
Year :
GLP :
Test substance : other TS

Method :
An octanol-water partition coefficient for the material was estimated using the KOWWIN program (v1.66) by entering the structure of the material into the program using SMILES code. This program estimates the partition coefficient by summing the coefficients of all fragments of the molecule based on an empirical equation that has been validated. As the material is a salt, independent calculations were conducted for the cation and anion.

Result :
KOWWIN Program (v1.66) Results:
=====

CATION Log Kow(version 1.66 estimate): 0.13

SMILES : CCCCN(CCCC)(CC)CCCCCN(CCCC)(CCCC)(CC)
CHEM : BQAOH++ (charged form)
MOL FOR: C26 H58 N2
MOL WT : 398.77

TYPE	NUM	LOGKOW	FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	6	-CH3	[aliphatic carbon]	0.5473	3.2838
Frag	20	-CH2-	[aliphatic carbon]	0.4911	9.8220
Frag	2	>N<	[+5 valence; single bonds;no H attach]	-6.6000	-13.2000
Const			Equation Constant		0.2290

Log Kow = 0.1348

ANION Log Kow(version 1.66 estimate): -3.22

SMILES : CCOS(=O)(=O)[Na]
CHEM : Sodium monoethylsulfate
MOL FOR: C2 H5 O4 S1 Na1
MOL WT : 148.11

2. Physico-Chemical Data

Id 68052-49-3

Date 09.01.2005

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH3 [aliphatic carbon]	0.5473	0.5473
Frag	1	-CH2- [aliphatic carbon]	0.4911	0.4911
Frag	1	-O- [oxygen, aliphatic attach]	-1.2566	-1.2566
Frag	1	-O-SO2-O- [sulfate, linear]	1.3500	1.3500
Factor	1	S-O-{Na,K,Li} [coef*(1+0.3*(NUM-1))]	-4.5800	-4.5800
Const		Equation Constant		0.2290

Log Kow = -3.2192

Test substance

:

BQAES CASNO 68052-49-3

Conclusion

:

As the cationic material is a quaternary salt, it will remain charged at all pH values and will have an estimated log Kow of 0.13

As the anionic portion of the material is acidic, it will remain in the charged form at all but strongly acidic pH levels and is estimated to have a log Kow of -3.22 for the charged form.

Reliability

:

(2) valid with restrictions

Estimates conducted by a reliable method are assigned a reliability score of 2 (reliable with restrictions).

Flag

:

Critical study for SIDS endpoint

02.01.2005

(6)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in

: Water

Value

: >= 480 g/l at 20 °C

pH value

:

concentration

: at °C

Temperature effects

:

Examine different pol.

:

pKa

: at 25 °C

Description

:

Stable

:

Deg. product

:

Method

: other: measured

Year

:

GLP

:

Test substance

: as prescribed by 1.1 - 1.4

Method

:

It is known from production of the material that solutions with content of 48% BQAES can be produced, stored and piped during production.

Conclusion

:

This material is considered highly water soluble.

Reliability

:

(2) valid with restrictions

Flag

:

Critical study for SIDS endpoint

02.01.2005

(7)

3.1.1 PHOTODEGRADATION

Type : air
 Light source : Sun light
 Light spectrum : nm
 Relative intensity : based on intensity of sunlight

INDIRECT PHOTOLYSIS

Sensitizer : OH
 Conc. of sensitizer :
 Rate constant : $\text{cm}^3/(\text{molecule} \cdot \text{sec})$
 Degradation : % after

Method

:
 As this is an organic salt, it is necessary to consider both the cation and anion as the salt can easily dissociate

The structure was initially examined to determine if there was a chromophore that could absorb light energy at wavelengths above 295 nm. As there is not for either cation or anion, it was assumed that direct photolysis would be unimportant to the fate of the test material.

The APOWIN program was also run to determine an estimated rate of reaction with hydroxyl radical. This rate was used to estimate the half-life of BQAOH in the troposphere assuming a tropospheric hydroxyl radical concentration of 1,500,000 molecules hydroxy radical per cm^3 .

Result

:

AOP Program (v1.90) Results:

=====
 SMILES : CCCC(N(CCCC)(CC)CCCCCN(CCCC)(CC)CCCC
 CHEM : BQAOH
 MOL FOR: C26 H58 N2
 MOL WT : 398.77

----- SUMMARY (AOP v1.90): HYDROXYL RADICALS -----
 Hydrogen Abstraction = 98.3799 E-12 $\text{cm}^3/\text{molecule} \cdot \text{sec}$
 Reaction with N, S and -OH = 0.0000 E-12 $\text{cm}^3/\text{molecule} \cdot \text{sec}$
 Addition to Triple Bonds = 0.0000 E-12 $\text{cm}^3/\text{molecule} \cdot \text{sec}$
 Addition to Olefinic Bonds = 0.0000 E-12 $\text{cm}^3/\text{molecule} \cdot \text{sec}$
 Addition to Aromatic Rings = 0.0000 E-12 $\text{cm}^3/\text{molecule} \cdot \text{sec}$
 Addition to Fused Rings = 0.0000 E-12 $\text{cm}^3/\text{molecule} \cdot \text{sec}$

OVERALL OH Rate Constant = 98.3799 E-12 $\text{cm}^3/\text{molecule} \cdot \text{sec}$
 HALF-LIFE = 0.109 Days (12-hr day; 1.5E6 OH/ cm^3)
 HALF-LIFE = 1.305 Hrs

AOP Program (v1.90) Results:

=====
 SMILES : CCOS(=O)(=O)O[Na]
 CHEM : Sodium monoethylsulfate
 MOL FOR: C2 H5 O4 S1 Na1
 MOL WT : 148.11

----- SUMMARY (AOP v1.90): HYDROXYL RADICALS -----
 Hydrogen Abstraction = 0.8211 E-12 $\text{cm}^3/\text{molecule} \cdot \text{sec}$
 Reaction with N, S and -OH = 0.0000 E-12 $\text{cm}^3/\text{molecule} \cdot \text{sec}$
 Addition to Triple Bonds = 0.0000 E-12 $\text{cm}^3/\text{molecule} \cdot \text{sec}$

3. Environmental Fate and Pathways

Id 68052-49-3

Date 09.01.2005

Addition to Olefinic Bonds = 0.0000 E-12 cm³/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm³/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm³/molecule-sec

OVERALL OH Rate Constant = 0.8211 E-12 cm³/molecule-sec
HALF-LIFE = 13.027 Days (12-hr day; 1.5E6 OH/cm³)

Test substance

:

BQAES CASNO 68052-49-3

Conclusion

:

Although vaporization into the atmosphere is considered unlikely, a value of approximately 1.3 hours is accepted as the atmospheric half-life of BQAES cation in the troposphere due to indirect photolysis and a value of approximately 13 days is accepted as the atmospheric half-life of BQAES anion in the troposphere due to indirect photolysis. No direct photolysis or reaction with atmospheric ozone is anticipated.

The calculated half-life of the cation is 1.3 hours based on 1,500,000 molecules of hydroxyl radical per cc.

The calculated half-life of the anion is 13 days based on 1,500,000 molecules of hydroxyl radical per cc.

Reliability

:

(2) valid with restrictions

Flag

:

Critical study for SIDS endpoint

02.01.2005

(2)

3.1.2 STABILITY IN WATER

Type

:

abiotic

t1/2 pH4

:

at °C

t1/2 pH7

:

at °C

t1/2 pH9

:

at °C

Deg. product

:

Method

:

Year

:

GLP

:

Test substance

:

as prescribed by 1.1 - 1.4

Method

:

Estimation on chemical principles for cation, literature value for anion.

Result

:

The enthalpy of reaction for hydrolysis of quaternary amine to tertiary amine and alkyl alcohol is calculated by summing the strengths of bonds broken and subtracting the sum of the strengths of the bond formed. (Organic Chemistry by Peter Vollhardt, W.H. Freeman & Co, NY, NY 1987 pp71-73)

Bonds broken

Water O-H 497 kJ

N-C 350 kJ

Bonds formed

Alcohol C-OH -356 kJ

Total estimated enthalpy of reaction = +491 kJ/mole

For the hydrolytic reaction of sodium ethyl sulfate, standard bond energies are not available for the sulfur-oxygen bond in sulfate and the organic ester. Examination of the structure suggests that hydrolysis may occur at a reasonable rate. The hydrolysis rate of diethyl sulfate to ethanol and sulfate has been determined to be 1.15×10^{-4} /sec at 25 deg C (Can J Chem 44: 1728-30, 1966 as cited in HSBD) translates to a half-life of 1.7 hours at pH 7 (SRC, as cited in HSDB). The rate of hydrolysis will increase in both acidic and basic waters as the reaction is catalyzed under these conditions (Weisenberger K, Mayer D; Ullmann's Encycl Indust Chem. MY, NY: VCH Pub A8: 493-504 1987, as cited in HSDB). Although the hydrolysis rate of diethyl sulfate comprises two hydrolytic reactions, a half life of hours for the overall reaction indicates a half-life of less than 1 day for sodium ethyl sulfate.

Conclusion

Bond energies from Lide, Handbook of Chemistry 84th edition 2003-2004 section 9

: The hydrolysis of the quaternary nitrogen to a tertiary amine and an alcohol is thermodynamically very unfavorable with a delta G estimated from the delta H of reaction greater than +400 kJ/mole. This is predicted to be a very endothermic reaction and should occur only under conditions of very high temperature.

It can be concluded that the quaternary amine portion of BQAES is stable in water and has a hydrolysis half-life of greater than 1 year.

The ethyl sulfate anion will hydrolyze readily and is estimated to have a half-life of less than 1 day in the environment.

Reliability

: (2) valid with restrictions

Estimates calculated by a reliable method are assigned a reliability score of 2 (reliable with restrictions).

Flag

03.01.2005 : Critical study for SIDS endpoint (5)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media : other: air water soil sedement
Method : Calculation according Mackay, Level III
Year :

Method : Theoretical Distribution (Fugacity) of BQAES in the environment was estimated using the MackKay EQC level III model set to estimate distribution after equal release to water, air and soil. The EPIWIN model was allowed to estimate physicochemical and fate parameters used in the calculations; however, these were verified for appropriateness before the final calculation was accepted. Because BQAES is a salt and is expected to dissociate in the environment, the cationic and anionic portions of the salt were independently modeled

3. Environmental Fate and Pathways

Id 68052-49-3
Date 09.01.2005

Result

:

Level III Fugacity Model (Full-Output):

=====
Chem Name : BQAOH and BQAES Cation
Molecular Wt: 398.77
Henry's LC : 5.15e-014 atm-m3/mole (Henrywin program)
Vapor Press : 1.73e-017 mm Hg (Mppbwin program)
Liquid VP : 1.37e-014 mm Hg (super-cooled)
Melting Pt : 318 deg C (Mppbwin program)
Log Kow : 0.13 (Kowwin program)
Soil Koc : 0.553 (calc by model)

	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	1.72e-010	2.61	0
Water	99.8	208	1000
Soil	1.15e-009	208	0
Sediment	0.15	832	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	3.69e-030	1.05e-007	3.97e-009	1.05e-008	3.97e-010
Water	1.49e-019	769	231	76.9	23.1
Soil	6.09e-029	8.86e-009	0	8.86e-010	0
Sedi	1.11e-019	0.29	0.00696	0.029	0.000696

Persistence Time: 231 hr
Reaction Time: 301 hr
Advection Time: 1e+003 hr
Percent Reacted: 76.9
Percent Advected: 23.1

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):

Air: 2.609
Water: 208.1
Soil: 208.1
Sediment: 832.3
Biowin estimate: 3.511 (days-weeks)

Advection Times (hr):

Air: 100
Water: 1000
Sediment: 5e+004

Level III Fugacity Model (Full-Output):

=====
Chem Name : Sodium monoethylsulfate
Molecular Wt: 148.11
Henry's LC : 1.08e-008 atm-m3/mole (Henrywin program)
Vapor Press : 1.94e-009 mm Hg (Mppbwin program)
Liquid VP : 1.04e-007 mm Hg (super-cooled)
Melting Pt : 200 deg C (Mppbwin program)
Log Kow : -3.22 (Kowwin program)
Soil Koc : 0.000247 (calc by model)

	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.000177	313	0

3. Environmental Fate and Pathways

Id 68052-49-3

Date 09.01.2005

Water	99.8	360	1000
Soil	0.00289	360	0
Sediment	0.166	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.03e-016	0.00134	0.00605	0.000134	0.000605
Water	1.25e-013	658	342	65.8	34.2
Soil	1.34e-016	0.0191	0	0.00191	0
Sedi	1.04e-013	0.274	0.0114	0.0274	0.00114

Persistence Time: 342 hr
Reaction Time: 520 hr
Advection Time: 1e+003 hr
Percent Reacted: 65.8
Percent Adverted: 34.2

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):

Air: 312.7
Water: 360
Soil: 360
Sediment: 1440
Biowin estimate: 2.872 (weeks)

Advection Times (hr):

Air: 100
Water: 1000
Sediment: 5e+004

Test substance : BQAES CASNO 68052-49-3

Conclusion : If released into water, the material remains primarily in the water column.

Reliability : (2) valid with restrictions

Estimates calculated by a reliable method are assigned a reliability score of 2 (reliable with restrictions).

Flag : Critical study for SIDS endpoint

04.01.2005 (3)

3.5 BIODEGRADATION

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

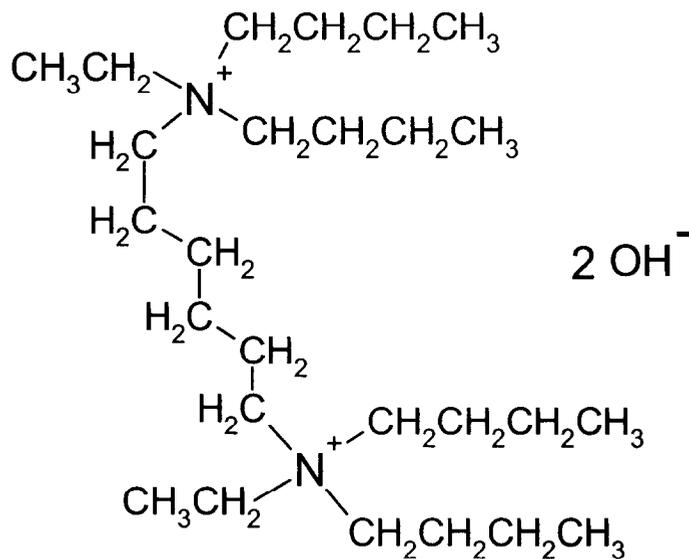
5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

- (1) Calculated by Toxicology and Regulatory Affairs, December 2004.
- (2) Calculated using EPIWIN 3.05 by Toxicology and Regulatory Affairs, December 2004
- (3) Calculated using EPIWIN 3.05 by Toxicology and Regulatory Affairs, December 2004
- (4) Calculated using MPBPWIN (v1.40) Program as found in EPIWIN 3.05 (2000, EPA version) by Toxicology and Regulatory Affairs, December 2004
- (5) Estimation conducted by Toxicology and Regulatory Affairs, December 2004.
- (6) Estimation conducted using KOWWIN Program (v1.66) as found in EPIWIN 3.05, Syracuse Research Corporation, ES EPA Version 2000, calculation by Toxicology and Regulatory Affairs, December 2004.
- (7) Solitia MSDS #068052493 for BQAES 45 - 97 % Aqueous Solution. 21 September 1998.

201-15773B2

HPV Data Set



RECEIVED
ORP/1/04/0
04 JAN 13 PM 12:41

BQAOH

Existing Chemical : ID: 111960-92-0
CAS No. : 111960-92-0
Product name : BQAOH
TSCA Name : 1,6-Hexanediaminium, N,N,N',N'-tetrabutyl-N,N'-diethyl-,dihydroxide

Producer related part

Company : Solutia Inc
Creation date : 10.01.2004

Substance related part

Company : Toxicology and Regulatory Affairs
Creation date : 10.01.2004

Status :
Memo : Prepared by:
Toxicology and Regulatory Affairs
Freeburg IL 62243
rauckman@toxicsolutions.com

Printing date : 09.01.2005
Revision date :
Date of last update : 04.01.2005

Number of pages : 22

Chapter (profile) :
Reliability (profile) :
Flags (profile) :

1. General Information

Id 111960-92-0
Date 09.01.2005

1.0.1 APPLICANT AND COMPANY INFORMATION

Type : manufacturer
Name : Solutia Inc
Contact person :
Date :
Street :
Town :
Country :
Phone :
Telefax :
Telex :
Cedex :
Email :
Homepage :

10.01.2004

1.2 SYNONYMS AND TRADENAMES

2. Physico-Chemical Data

Id 111960-92-0

Date 09.01.2005

2.1 MELTING POINT

Value : ca. 0 - -3.2 °C
Sublimation :
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4

Method :
The material as produced is an aqueous solution containing up to 25% BQAOH. The practical freezing point of the solution is a function of the solvent's freezing point and the freezing point depression caused by the solute. An approximate freezing point can be calculated based on the molal freezing-point depression constant for water of 1.86°C

Result :
For a 25% solution of BQAOH in water the approximate molality is 0.577. Considering that there could be up to three ions, the freezing point depression could be as great as 3.21°C.

Conclusion :
The freezing point range for this material as an aqueous solution is 0 to -3.2°C; however, limits on the solubility could cause precipitated solid formation prior to freezing.

Reliability : (2) valid with restrictions
Estimates calculated by a reliable method are assigned a reliability score of 2.

Flag : Critical study for SIDS endpoint
10.01.2004

Value : <= 380 °C
Sublimation :
Method : other: calculated
Year :
GLP :
Test substance : other TS

Method :
This material is produced, handled and disposed of as an aqueous solution containing up to 25% organic content. The melting point for the solid material has not been recorded as it is not isolated, but as an impure salt it is expected to be relatively high and variable. For the purpose of an HPV program, the melting point of the solid was estimated with the MPBPWIN (v 1.4) program. This estimate is considered an upper limit of the practical melting point for the solid.

Result :
MPBPWIN (v1.40) Program Results:
=====
Experimental Database Structure Match: no data

SMILES : CCCC(CCCC)(CC)CCCCCN(CCCC)(CCCC)(CC)
CHEM : BQAOH++ (twice charged form)
MOL FOR: C26 H58 N2
MOL WT : 398.77

2. Physico-Chemical Data

Id 111960-92-0
Date 09.01.2005

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	6	-CH3	-5.10	-30.60
Group	20	-CH2-	11.27	225.40
Group	2	>N< (+5)	340.00	680.00
*		Equation Constant		122.50

RESULT	MELTING POINT in deg Kelvin	997.30
RESULT-limit	MELTING POINT in deg Kelvin	623.00
	MELTING POINT in deg C	349.84

Melting Point: 349.84 deg C (Adapted Joback Method)
Melting Point: 309.98 deg C (Gold and Ogle Method)
Mean Melt Pt : 329.91 deg C (Joback; Gold,Ogle Methods)
Selected MP: 317.95 deg C (Weighted Value)

Test substance :
Conclusion : Solid portion of BQAOH solution as produced.
Reliability : The actual melting point of the solid portion of this material is expected to vary, depending on the impurity level, with a maximum of 318 °C
(2) valid with restrictions
Estimates calculated by a reliable method are assigned a reliability score of 2.
Flag : Critical study for SIDS endpoint
02.01.2005 (10)

2.2 BOILING POINT

Value : ca. 100 - 101 °C at 1013 hPa
Decomposition :
Method : other: calculated
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Method :
The material as produced is an aqueous solution containing up to 25% BQAOH. The practical boiling point of the solution is a function of the solvent's boiling point and the boiling point elevation caused by the solute. An approximate boiling point can be calculated based on the molal boiling-point elevation constant for water of 0.52°C/m.
Remark :
The solid material is expected to decompose before boiling as it is a high molecular weight salt.
Result :
For a 25% solution of BQAOH in water, the approximate molality is 0.577. Considering that there could be up to three ions, the boiling-point elevation could be as great as 0.9°C.
Conclusion :
The initial boiling point range for this material as an aqueous solution is 100

2. Physico-Chemical Data

Id 111960-92-0
Date 09.01.2005

Reliability : to 101°C.
: (2) valid with restrictions

Estimates calculated by a reliable method are assigned a reliability score of 2.

Flag : Critical study for SIDS endpoint
10.01.2004

2.3 DENSITY

2.4 VAPOUR PRESSURE

Value : < .000000000001 hPa at 25 °C
Decomposition :
Method : other (calculated): EPIWIN
Year :
GLP :
Test substance : other TS

Method :

The vapor pressure for a charged salt is expected to be negligible. In addition, as this material is produced and handled as an aqueous solution, the Henry's law constant is a more important factor for exposure consideration from bulk material or material that is introduced into the water column. EPIWIN was used to provide estimates for both the vapor pressure and the Henry's law constant. EPIWIN was also used to estimate the half live for volatilization from water in a model river.

Result :

MPBPWIN (v1.40) Program Results:
=====
Experimental Database Structure Match: no data

SMILES : CCCC(CCCC)(CC)CCCCCN(CCCC)(CCCC)(CC)
CHEM : BQAOH++ (twice charged form)
MOL FOR: C26 H58 N2
MOL WT : 398.77

----- SUMMARY MPBPWIN v1.40 -----
Vapor Pressure Estimations (25 deg C):
(Using BP: 725.54 deg C (estimated))
(Using MP: 317.95 deg C (estimated))
VP: 8.95E-026 mm Hg (Antoine Method)
VP: 1.73E-017 mm Hg (Modified Grain Method)
VP: 8.8E-017 mm Hg (Mackay Method)
Selected VP: 1.73E-017 mm Hg (Modified Grain Method)

HENRY (v3.10) Program Results:
=====

Bond Est : 5.15E-014 atm-m3/mole
Group Est: Incomplete

SMILES : CCCC(CCCC)(CC)CCCCCN(CCCC)(CCCC)(CC)
CHEM : BQAOH++ (twice charged form)
MOL FOR: C26 H58 N2
MOL WT : 398.77

2. Physico-Chemical Data

Id 111960-92-0

Date 09.01.2005

----- HENRYWIN v3.10 Results -----

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN FRAGMENT	58 Hydrogen to Carbon (aliphatic) Bonds		-6.9413
FRAGMENT	19 C-C		2.2098
FRAGMENT	8 C-N		10.4080
FACTOR	* Quaternary ammonium-type cmpd	ESTIMATE	6.0000
RESULT	BOND ESTIMATION METHOD for LWAPC VALUE	TOTAL	11.676

HENRYs LAW CONSTANT at 25 deg C = 5.15E-014 atm-m3/mole
= 2.11E-012 unitless

Henrys LC [VP/WSol estimate using EPI values]:

HLC: 3.796E-021 atm-m3/mole

VP: 1.73E-017 mm Hg

WS: 2.39E+003 mg/L

-----VOLATIZATION FROM WATER-----

	RIVER	LAKE
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05
HALF-LIFE (hours) :	2.27E+010	2.477E+011
HALF-LIFE (days) :	9.459E+008	1.032E+010
HALF-LIFE (years) :	2.59E+006	2.825E+007

Test substance : Solid portion of BQAOH solution as produced.

Conclusion : The estimated vapor pressure is negligible at 2.2E-17 hPa

Reliability : (2) valid with restrictions

Estimates calculated by a reliable method are assigned a reliability score of 2.

Flag : Critical study for SIDS endpoint

10.01.2004 (11)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water

Log pow : ca. .13 at 25 °C

pH value :

Method : other (calculated): EPIWIN

Year :

GLP :

Test substance : other TS

Method : An octanol-water partition coefficient for the material was estimated using the KOWWIN program (v1.66) by entering the structure of the material into the program using SMILES code. This program estimates the partition coefficient by summing the coefficients of all fragments of the molecule based on an empirical equation that has been validated.

2. Physico-Chemical Data

Id 111960-92-0
Date 09.01.2005

Result : KOWWIN Program (v1.66) Results:

=====

Log Kow(version 1.66 estimate): 0.13

SMILES : CCCCN(CCCC)(CC)CCCCCN(CCCC)(CCCC)(CC)
CHEM : BQAOH++ (charged form)
MOL FOR: C26 H58 N2
MOL WT : 398.77

TYPE	NUM	LOGKOW	FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	6	-CH3	[aliphatic carbon]	0.5473	3.2838
Frag	20	-CH2-	[aliphatic carbon]	0.4911	9.8220
Frag	2	>N<	[+5 valence; single bonds;no H attach]	-6.6000	-13.2000
Const			Equation Constant		0.2290

Log Kow = 0.1348

Test substance : BQAOH CASNO 111960-92-0 (as smiles notation)

Conclusion : As the cationic material is a quaternary salt, it will remain charged at all pH values and will have an estimated log Kow of 0.13

Reliability : (2) valid with restrictions

Estimates calculated by a reliable method are assigned a reliability score of 2 (reliable with restrictions).

Flag : Critical study for SIDS endpoint
02.01.2005 (8)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : ≥ 280 g/l at 20 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description : very soluble (> 10000 mg/L)
Stable :

Remark : It is know from production and testing of the material that solutions with content of 28 % BQAOH can be produced and shipped for toxicity testing. In addition the MSDS specification allows for solutions concentrated as 25% by weight.

Conclusion : This material is considered highly water soluble.

Reliability : (2) valid with restrictions

Information obtained by a scientifically defensible method.

Flag : Critical study for SIDS endpoint
10.01.2004 (9)

3.1.1 PHOTODEGRADATION

Type : air
Light source : Sun light
Light spectrum : nm
Relative intensity : based on intensity of sunlight

DIRECT PHOTOLYSIS

Halflife t1/2 : ca. 1.3 hour(s)
Degradation : % after
Quantum yield :

INDIRECT PHOTOLYSIS

Sensitizer : OH
Conc. of sensitizer :
Rate constant : cm³/(molecule*sec)
Degradation : % after

Method :

The structure was initially examined to determine if there was a chromophore that could absorb light energy at wavelengths above 295 um. As there is not, it was assumed that direct photolysis would be unimportant to the fate of the test material.

The APOWIN program was also run to determine an estimated rate of reaction with hydroxyl radical. This rate was used to estimate the half-life of BQAOH in the troposphere assuming a tropospheric hydroxyl radical concentration of 1,500,000 molecules hydroxy radical per cm3.

Result :

The calculated half-life is 1.3 hours based on 1,500,000 molecules of hydroxyl radical per cc.

AOP Program (v1.90) Results:

=====

SMILES : CCCCN(CCCC)(CC)CCCCCN(CCCC)(CC)CCCC
CHEM : BQAOH
MOL FOR: C26 H58 N2
MOL WT : 398.77

----- SUMMARY (AOP v1.90): HYDROXYL RADICALS -----

Hydrogen Abstraction = 98.3799 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 98.3799 E-12 cm3/molecule-sec
HALF-LIFE = 0.109 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 1.305 Hrs

Conclusion :

Although vaporization into the atmosphere is considered unlikely, a value of approximately 1.3 hours is accepted as the atmospheric half-life of BQAOH in the troposphere due to indirect photolysis. No direct photolysis or reaction with atmospheric ozone is anticipated.

Reliability :

(2) valid with restrictions
Flag : Critical study for SIDS endpoint

02.01.2005

(3)

3.1.2 STABILITY IN WATER

Type	:	abiotic										
t1/2 pH4	:	at °C										
t1/2 pH7	:	at °C										
t1/2 pH9	:	at °C										
Deg. product	:											
Method	:											
Year	:											
GLP	:											
Test substance	:	as prescribed by 1.1 - 1.4										
Method	:	Estimation on chemical principles.										
Result	:	<p>The enthalpy of reaction for hydrolysis of quaternary amine to tertiary amine and alkyl alcohol is calculated by summing the strengths of bonds broken and subtracting the sum of the strengths of the bond formed. (Organic Chemistry by Peter Vollhardt, W.H. Freeman & Co, NY, NY 1987 pp71-73)</p> <table border="0"> <tr> <td colspan="2">Bonds broken</td> </tr> <tr> <td>Water O-H</td> <td>497 kJ</td> </tr> <tr> <td>N-C</td> <td>350 kJ</td> </tr> <tr> <td colspan="2">Bonds formed</td> </tr> <tr> <td>Alcohol C-OH</td> <td>-356 kJ</td> </tr> </table> <p>Total estimated enthalpy of reaction = +491 kJ/mole</p> <p>Bond energies from Lide, Handbook of Chemistry 84th edition 2003-2004 section 9</p>	Bonds broken		Water O-H	497 kJ	N-C	350 kJ	Bonds formed		Alcohol C-OH	-356 kJ
Bonds broken												
Water O-H	497 kJ											
N-C	350 kJ											
Bonds formed												
Alcohol C-OH	-356 kJ											
Conclusion	:	<p>The hydrolysis of the quaternary nitrogen to a tertiary amine and an alcohol is thermodynamically very unfavorable with a delta G estimated from the delta H of reaction to be greater than +400 kJ/mole. This is predicted to be a very endothermic reaction and should occur only under conditions of very high temperature.</p> <p>It can be concluded that the quaternary amine portion of BQAOH is stable in water and has a hydrolysis half-life of greater than 1 year.</p>										
Reliability	:	<p>(2) valid with restrictions</p> <p>Estimates calculated by a reliable method are assigned a reliability score of 2 (reliable with restrictions).</p>										
Flag	:	Critical study for SIDS endpoint										
02.01.2005		(2)										

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3. Environmental Fate and Pathways

Id 111960-92-0
Date 09.01.2005

3.3.2 DISTRIBUTION

Media : other: air water soil sedement
Method : Calculation according Mackay, Level III
Year :

Method :
Theoretical Distribution (Fugacity) of BQAOH in the environment was estimated using the MacKay EQC level III model set to estimate distribution after equal release to water, air and soil. The EPIWIN model was allowed to estimate physicochemical and fate parameters used in the calculations; however, these were verified for appropriateness before the final calculation was accepted. Because BQAOH is a salt and is expected to dissociate in the environment, the cationic portions were independently modeled.

Result :
Level III Fugacity Model (Full-Output):

=====
Chem Name : BQAOH and BQAES Cation
Molecular Wt: 398.77
Henry's LC : 5.15e-014 atm-m3/mole (Henrywin program)
Vapor Press : 1.73e-017 mm Hg (Mppbwin program)
Liquid VP : 1.37e-014 mm Hg (super-cooled)
Melting Pt : 318 deg C (Mppbwin program)
Log Kow : 0.13 (Kowwin program)
Soil Koc : 0.553 (calc by model)

	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	1.72e-010	2.61	0
Water	99.8	208	1000
Soil	1.15e-009	208	0
Sediment	0.15	832	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	3.69e-030	1.05e-007	3.97e-009	1.05e-008	3.97e-010
Water	1.49e-019	769	231	76.9	23.1
Soil	6.09e-029	8.86e-009	0	8.86e-010	0
Sedi	1.11e-019	0.29	0.00696	0.029	0.000696

Persistence Time: 231 hr
Reaction Time: 301 hr
Advection Time: 1e+003 hr
Percent Reacted: 76.9
Percent Advected: 23.1

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 2.609
Water: 208.1
Soil: 208.1
Sediment: 832.3
Biowin estimate: 3.511 (days-weeks)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

3. Environmental Fate and Pathways

Id 111960-92-0
Date 09.01.2005

Test substance : BQAOH CASNO 111960-92-0 (as smiles notation)
Conclusion : If released into water, the material remains primarily in the water column.
Reliability : (2) valid with restrictions
Estimates calculated by a reliable method are assigned a reliability score of 2 (reliable with restrictions).
Flag : Critical study for SIDS endpoint
04.01.2005 (4)

3.5 BIODEGRADATION

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

5.1.1 ACUTE ORAL TOXICITY

Type : LD50
 Value : = 350 mg/kg bw
 Species : rat
 Strain : Sprague-Dawley
 Sex : male/female
 Number of animals :
 Vehicle : other: Dosed as produced (28% solution in water)
 Doses :
 Method :
 Year :
 GLP : yes
 Test substance : as prescribed by 1.1 - 1.4

Method :
 Groups of five young adult Sprague-Dawley male rats of each sex were administered test material by intragastric intubation as received. The test material was accompanied by a sample identification sheet specifying that the test material was "28% pure". It is assumed that the remainder was water, consistent with the product description in other literature. At dosing, average group weight of males was 200 to 220 g and average group weight of females was 185-210 grams. Surviving animals were observed for 14 days and were sacrificed and necropsied.

Result :
 Dose levels and results are given in the table

MALES

Dose	As	Mortality	Time of Death
28% soln	BQAOH		
2,000	560	5/5	30 -120 min
1,580	442	4/5	30 -120 min
1,260	315	2/5	120 min
1,000	280	1/5	30 min
794	222	0/5	-

FEMALES

Dose	As	Mortality	Time of Death
28% soln	BQAOH		
2,000	560	5/5	30 -120 min
1,580	442	5/5	120 min
1,260	315	4/5	30 - 120 min
1,000	280	1/5	120 min
794	222	0/5	-

CLINICAL EFFECTS:

@ Lethal Doses: Lethargy, rapidly increasing weakness, collapse and death.

@ Nonlethal Doses: Lethargy lasting 1 day.

GROSS NECROPSY FINDINGS

Decedents: Hemorrhagic lung and liver, liver discoloration in some cases, one animal showed kidney discoloration, gastrointestinal inflammation.

Survivors: Viscera appeared normal at sacrifice.

Conclusion : BQAOH has an acute oral LD50 in Sprague-Dawley rats of 1250 mg/kg (95% CI 1120- 1380) based on the 28% solution. As a pure material it has an LD50 of 350 mg/kg (95% CI 314-386). Male and female rats are approximately equally sensitive.

Reliability : (1) valid without restriction
Study protocol was comparable to current OECD guideline, study conducted under GLP.

Flag : Critical study for SIDS endpoint
24.01.2004

(14)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50
Value : = 22.4 mg/kg bw
Species : rabbit
Strain : New Zealand white
Sex : male/female
Number of animals :
Vehicle : other: Applied as produced (28% water solution)
Doses :
Method :
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Method :
Groups of two New Zealand albino rabbits of each sex were dermally exposed to undiluted test material at 6 closely spaced dose levels. At each dose level, one animal's skin was abraded and the other's skin was left intact. The test material remained in contact with the skin for 24 hours and was then removed.

The test material was accompanied by a sample identification sheet specifying that the test material was "28% pure". It is assumed that the remainder was water, consistent with the description of the product in other literature. Surviving animals were observed for 14 days then were sacrificed and necropsied.

Result : Dose levels and mortality results are given in the table

MALES

Dose	As	Mortality		Time of
28% soln	BQAOH	intact	abraded	Death
50.1	14.0	0/1	0/1	-
63.1	17.7	1/1	0/1	2 hours
79.4	22.2	0/1	0/1	-
100.0	28.0	1/1	1/1	2 hours
126.0	35.3	1/1	1/1	2 hours
158.0	44.2	1/1	1/1	2 hours

FEMALES

Dose	As	Mortality		Time of
28% soln	BQAOH	intact	abraded	Death
50.1	14.0	0/1	0/1	-
63.1	17.7	0/1	1/1	24 hours
79.4	22.2	1/1	0/1	2 hours
100.0	28.0	1/1	1/1	2 hours
126.0	35.3	0/1	1/1	2 hours
158.0	44.2	1/1	1/1	2 hours

CLINICAL EFFECTS:

@ Lethal Doses: Rapidly increasing weakness, collapse and death.

@ Nonlethal Doses: Not reported.

GROSS NECROPSY FINDINGS

Decedents: Hemorrhagic areas of lung, liver discoloration in one animal, two animals showed enlarged gall bladders.

Survivors: Viscera appeared normal at sacrifice.

Conclusion : BQAOH is very toxic to rabbits by the dermal route with an acute dermal LD50 in rabbits of 80 mg/kg (95% CI 67 - 94) based on the 28% solution. As a pure material it has an LD50 of 22.4 mg/kg (95% CI 18.8 - 26.3). Males and females have approximately equal sensitivity.

Reliability : (1) valid without restriction

Although the number of animals per group was low, sufficient data were generated by a scientifically defensible method, using GLP conditions, to consider this a reliable estimate of dermal toxicity.

Flag : Critical study for SIDS endpoint
24.01.2004

(14)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

Type : Chronic
Species : rat
Sex : male/female
Strain : Sprague-Dawley
Route of admin. : oral feed
Exposure period : 104 Weeks
Frequency of treatm. : Cont
Post exposure period :
Doses : 300, 750 or 1500 ppm
Control group : yes, concurrent vehicle
NOAEL : = 750 ppm
Method :
Year :
GLP : no data
Test substance : other TS

Method :
 Test substance was fed in diet to 60 Sprague-Dawley CD rats/sex/group for 104 weeks at 0 (Ground Purina Certified Rodent Chow # 5002), 300, 750, or 1500 ppm. Two control groups were included and treated as independent entities.

Result :
 Chronic NOEL = 750 ppm (Decreased bodyweight, bodyweight gain and food consumption was observed in each sex at 1500 ppm. Increased incidence in mesenteric lymph node pathology (blood in sinuses, hemosiderosis and histiocytosis) occurred in both sexes at 1500 ppm. Bile duct hyperplasia occurred in females at 1500 ppm.) Treatment-related oncogenicity was not observed. No adverse oncogenic effects were observed, however, there were treatment-related changes in both sexes in the mesenteric lymph node (blood filled sinuses, hemosiderosis & hystiocytosis) and bile duct hyperplasia at 1500 ppm.

Test substance :
 Bardac 2280 (didecyldimethylammonium chloride, CASNO 7173-51-5), 80.8% pure

Reliability : (2) valid with restrictions
 Study judged as "acceptable" by California EPA for establishing pesticide tolerance

Flag : Critical study for SIDS endpoint
 04.01.2005 (6)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : HGPRT assay
System of testing : CHO Cells
Test concentration :
Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method :
Year :

5. Toxicity

Id 111960-92-0
Date 09.01.2005

GLP	:	no data	
Test substance	:	other TS	
Method	:		
		Test material was assayed in a CHO/HGPRT forward mutation assay at concentrations of 0 (vehicle = deionized water), 3.0, 4.0, 5.0, 6.0, 7.0, 8.0 and 10.0 µg/ml without metabolic activation.	
Result	:		
		In the first trial, the survival ranged from 105.9% to 10.7%. The second trial gave survivals ranging from 106.6% to 5.7%. Neither assay showed an increase in mutant frequency. Trials with metabolic activation were conducted at concentrations of 0, 1.0, 5.0, 10.0, 13.0, 15.0, 18.0, 20.0, 22.0 and 25.0 µg/ml. The first trial yielded survivals of 105.1% to 2.8% (at doses from 5.0 to 25.0 µg/ml). The repeat trial yielded survivals from 102.4% to 19.3% (at doses from 10.0 to 22.0 µg/ml).	
		Neither trial showed an increase in mutant frequency.	
Test substance	:		
		Bardac 2280 (didecyldimethylammonium chloride, CASNO 7173-51-5), 80% B-1889	
Reliability	:	(2) valid with restrictions	
		Study judged as "acceptable" by California EPA for establishing pesticide tolerance	
Flag	:	Critical study for SIDS endpoint	
04.01.2005			(12)
Type	:	Cytogenetic assay	
System of testing	:	CHO Cells	
Test concentration	:		
Cycotoxic concentr.	:		
Metabolic activation	:	with and without	
Result	:	negative	
Method	:		
Year	:		
GLP	:	no data	
Test substance	:	other TS	
Method	:		
		A 50% solution of didecyldimethylammonium chloride was tested in an in vitro cytogenetic assay in the presence of activation (+S9) with Chinese Hamster ovary cells in duplicate at concentrations of untreated, 0 (deionized distilled water), 2, 4, 8, and 16 µg/ml. In the absence of activation (no S9), concentrations for the first replicate were untreated, 0 (deionized distilled water), 0.25, 0.5, 1.0, and 2.0 µg/ml. These levels did not produce the expected toxicity and levels for the second replicate were increased to: untreated, 0, 1.0, 2.0, 4.0, and 8.0 µg/ml.	
Result	:		
		No adverse effects either with or without S9	
Test substance	:		
		Bardac 2280 (didecyldimethylammonium chloride, CASNO 7173-51-5), 50% in water tested as PO151	
Reliability	:	(2) valid with restrictions	
		Study judged as "acceptable" by California EPA for establishing pesticide tolerance	
Flag	:	Critical study for SIDS endpoint	
04.01.2005			(5)

5.6 GENETIC TOXICITY 'IN VIVO'

Type : Cytogenetic assay
Species : rat
Sex : male/female
Strain : Crj: CD(SD)
Route of admin. : gavage
Exposure period : 6, 24 or 48 hours
Doses : 600 mg/kg
Result : negative
Method :
Year :
GLP : no data
Test substance : other TS

Method :
 The test substance was administered by gavage to CD albino rats (5/sex/sampling time) at 0 (distilled water) and 600 mg/kg. Bone marrow sampling of vehicle control and test substance groups was performed at 6, 24, and 48 hours. The positive control, cyclophosphamide (40 mg/kg), was sampled at 24 hours.

Result :
 No treatment-related effects to metaphase chromosomes were observed.

Positive controls gave the expected result.

Test substance :
 Didecyldimethylammonium chloride, CASNO 7173-51-5, 50.3% solution

Reliability : (2) valid with restrictions
 Study judged as "acceptable" by California EPA for establishing pesticide tolerance

Flag : Critical study for SIDS endpoint
 04.01.2005

(1)

5.8.1 TOXICITY TO FERTILITY

Type : Two generation study
Species : rat
Sex : male/female
Strain : Sprague-Dawley
Route of admin. : oral feed
Exposure period :
Frequency of treatm. : Cont
Premating exposure period
 Male : 10 weeks
 Female : 10 weeks
Duration of test :
No. of generation studies : 2
Doses : 300, 750 or 1500 ppm
Control group : yes, concurrent vehicle
NOAEL parental : = 750 ppm

5. Toxicity

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NOAEL F1 offspring	:	= 750 ppm
NOAEL F2 offspring	:	= 750 ppm
Result	:	Not a specific reproductive toxin
Method	:	
Year	:	
GLP	:	no data
Test substance	:	other TS
Method	:	Didecyldimethylammoniumchloride (80.8% pure), was fed in diet to Sprague-Dawley (CD) rats (28/sex/dose) through two generations with 2 litters per generation at 0 (Purina Certified Ground Rodent Chow. #5002), 300, 750, or 1500 ppm. Treatment began 10 weeks prior to mating.
Result	:	Parental NOEL = 750 ppm (Reduced bodyweights and food consumption were observed at 1500 ppm). Reproductive NOEL = 750 ppm (Pups had reduced bodyweight gain at 1500 ppm).
Test substance	:	Didecyldimethylammoniumchloride, CASNO 7173-51-5 (80.8% pure)
Reliability	:	(2) valid with restrictions Study judged as "acceptable" by California EPA for establishing pesticide tolerance
Flag	:	Critical study for SIDS endpoint
04.01.2005		(13)

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rabbit
Sex	:	
Strain	:	New Zealand white
Route of admin.	:	gavage
Exposure period	:	day 6 - 18 of gestation
Frequency of treatm.	:	daily
Duration of test	:	
Doses	:	1, 3 or 10 mg/kg-day
Control group	:	yes, concurrent vehicle
NOAEL maternal tox.	:	= 1 mg/kg bw
NOAEL teratogen.	:	mg/kg bw
other: NOEL	:	= 3
Developmental		
Method	:	Test material was administered by gavage to mated New Zealand White rabbits on days 6 - 18 of gestation (day of mating = day 0 of gestation) at 0 (vehicle = deionized water), 1.0, 3.0 or 10.0 mg/kg/day (16/group).
Result	:	Maternal NOEL = 1.0 mg/kg (4 deaths accompanied by labored respiration, gasping, sloughing of esophageal lining and stomach, and decreased weight gain was observed at 10.0 mg/kg. At 3.0 mg/kg audible respiration, hypoactivity and decreased weight gain was observed.)

5. Toxicity

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Test substance : Developmental NOEL = 3.0 mg/kg (An increased number of dead fetuses/litter and decreased fetal body weight at 10.0 mg/kg was observed.)
Bardac 2280 (didecyldimethylammonium chloride, CASNO 7173-51-5), 80.8% pure, Batch B-1889

Reliability : (2) valid with restrictions

Flag : Study judged as "acceptable" by California EPA for establishing pesticide tolerance
04.01.2005 : Critical study for SIDS endpoint (7)

- (1) Analysis of Metaphase Chromosomes Obtained from Bone Marrow of Rats Treated with P0151", (J.A. Allen, R.J. Proudlock & P.C. Brooker, Huntingdon Research Center, Huntingdon, England, Project # LZA 24/8761, 4/1/87). As cited in; California EPA Dept of Pesticide Regulation Medical Toxicology Branch. Summary of Toxicology Data Didecyldimethylammoniumchloride revised 2/14/1996. <http://www.cdpr.ca.gov/docs/toxsums/pdfs/1682.pdf>
- (2) Calculated by Toxicology and Regulatory Affairs, December 2004
- (3) Calculated using EPIWIN 3.05 by Toxicology and Regulatory Affairs, October 2004
- (4) Calculated using EPIWIN 3.05 by Toxicology and Regulatory Affairs, October 2004
- (5) Chromosomal Aberrations Assay with Chinese Hamster Ovary Cells in vitro", (M. Holmstrom, D.J. Leftwich & I.A. Leddy, Gulland Laboratories of Inveresk Research International, Musselburgh, Scotland, Report # 4236, October 1986). As cited in; California EPA Dept of Pesticide Regulation Medical Toxicology Branch. Summary of Toxicology Data Didecyldimethylammoniumchloride revised 2/14/1996. <http://www.cdpr.ca.gov/docs/toxsums/pdfs/1682.pdf>
- (6) Chronic Dietary Toxicity/Oncogenicity Study with Didecyldimethylammoniumchloride in Rats", (M.W. Gill, J.S. Chun & C.L. Wagner, Bushy Run Research Center, Export, PA., Report # 53-566, 6/27/91). As cited in; California EPA Dept of Pesticide Regulation Medical Toxicology Branch. Summary of Toxicology Data Didecyldimethylammoniumchloride revised 2/14/1996. <http://www.cdpr.ca.gov/docs/toxsums/pdfs/1682.pdf>
- (7) Developmental Toxicity Study of Didecyldimethyl ammonium chloride Administered by Gavage to New Zealand White Rabbits," (Tyl, R.W., Bushy Run Research Center, Project ID 51-590, 1-27-89). As cited in; California EPA Dept of Pesticide Regulation Medical Toxicology Branch. Summary of Toxicology Data Didecyldimethylammoniumchloride revised 2/14/1996. <http://www.cdpr.ca.gov/docs/toxsums/pdfs/1682.pdf>
- (8) Estimation conducted using KOWWIN Program (v1.66) as found in EPIWIN 3.05, Syracuse Research Corporation, ES EPA Version 2000, calculation by Toxicology and Regulatory Affairs, December 2003.
- (9) Material Safety Data Sheet, BQAOH, Solutia MSDS No.: 0656523448 September 2, 1998
- (10) MPBPWIN (v1.40) program as found in EPIWIN 3.05, Syracuse Research Corporation, ES EPA Version 2000
- (11) MPBPWIN (v1.40), HENRY and Volatilization programs as found in EPIWIN 3.05, Syracuse Research Corporation, ES EPA Version 2000
- (12) Mutagenicity Test on Didecyldimethylammoniumchloride (DDAC) in the CHO/HGPRT Forward Mutation Assay" (Young, R.R., Hazleton Laboratories America, Inc., Study No. 10141-0-435, 9-9-88). As cited in; California EPA Dept of Pesticide Regulation Medical Toxicology Branch. Summary of Toxicology Data Didecyldimethylammoniumchloride revised 2/14/1996. <http://www.cdpr.ca.gov/docs/toxsums/pdfs/1682.pdf>

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- (13) Two-Generation Reproduction Study in Sprague-Dawley (CD.) Rats with Didecyldimethylammoniumchloride Administered in the Diet", (T.L. Neepier-Bradley, Bushy Run Research Center, Export, PA., Report # 52-648, 2/1/91). As cited in; California EPA Dept of Pesticide Regulation Medical Toxicology Branch. Summary of Toxicology Data Didecyldimehylammoniumchloride revised 2/14/1996.
<http://www.cdpr.ca.gov/docs/toxsums/pdfs/1682.pdf>
- (14) Younger Laboratories Inc, Final Report: Acute Toxicity Testing of BQAOH, project YO-81-063, 11-6-1981; sponsored by Monsanto Co.