

APPENDIX E GOLDER SUPPORTING HAZARD RANKING INFORMATION



Name	2-Methyl-4-Isothiazolin-3-one
Synonyms	2-Methyl-3(2H)-isothiazolone
CAS number	2682-20-4
Molecular formula	C ₄ H ₅ N ₁ O ₁ S ₁
Product name	M275

Physical Properties	Value	Reference
Phase/state	NA	
Molecular weight	115.15 g/mol	EPISUITE
Melting point	47.48 °C	EPISUITE
Boiling point	237.75 °C	EPISUITE
Density/ specific gravity	NA	
Vapour pressure	0.031 mm Hg at 25°C	EPISUITE
Solubility	5.367 x 10 ⁵ mg/L	EPISUITE
Henrys law constant	4.96 x 10 ⁻⁸ atm m ³ /mole (BOND Method)	EPISUITE
Organic carbon partition coefficient (koc)	12.08 (MCI Method)	EPISUITE
Log organic carbon partition coefficient (log Koc)	1.082 (MCI Method)	EPISUITE
Log octanol-water partition coefficient (log Kow)	-0.83	EPISUITE

Persistence/ Bioaccumulation	Value	Reference
Aquatic biodegradation	NA	
Aerobic BOD	NA	
Anaerobic BOD	NA	
Biowin7 (Anerobic linear model)	Biodegrades fast	EPISUITE
Fugacity		
Air %	0.519	EPISUITE
Water %	34.1	EPISUITE
Soil %	65.3	EPISUITE
Sediment %	0.0797	EPISUITE
Bioconcentration factor (BCF)	3.162 L/kg wet wt	EPISUITE
Biotransformation half-life	0.02263 days	EPISUITE

Notes: 1 EPI Suite™ v4.0, United States Environmental Protection Agency.
 NA - not available

Chemical Information Sheet - 2-Methyl-4-Isothiazolin-3-one

Aquatic toxicity guidelines				
Guideline	Year	Type	Value (g/m ³)	Notes
ANZECC	2000	Aquatic toxicity	NA	
USEPA	2006	Aquatic toxicity	NA	
Other water quality guidelines				
Guideline	Year	Type	Value (g/m ³)	Notes
ADWG	2004	Drinking water	NA	
NZDWS	2008	Drinking water	NA	
WHO	2006	Drinking water	NA	
USEPA	2006	Human Health	NA	
IARC	2006	Carcinogen risk	NA	Not listed on IARC database.
ANZECC	2000	Stock water	NA	

Aquatic Ecotoxicological Data

Acute toxicity data							
Species name	Common name	Endpoint	Effect	Effect measure	Test time (days)	Conc (µg/L)	Reference
Oncorhynchus mykiss	Rainbow Trout	LC50	MOR	MORT	4	70	ECOTOX
Daphnia magna	Water Flea	EC50	ITX	IMBL	2	180	ECOTOX
Oncorhynchus mykiss	Rainbow Trout	LC50	MOR	MORT	4	190	ECOTOX
Lepomis macrochirus	Bluegill	LC50	MOR	MORT	4	300	ECOTOX

Media Type : Freshwater for acute toxicity data

MOR/ MORT: Mortality

ITX: Intoxication

IMBL: Immobile

Notes: ANZECC, 2000: Australian and New Zealand guidelines for fresh and marine water quality. Australian and New Zealand Environment and Conservation Council.

USEPA, 2006: National recommended water quality criteria: 2006. EPA-822-R-02-047. Office of Water and Office of Science and Technology, United States Environmental Protection Agency.

ADWG, 2004: Australian drinking water guidelines . Endorsed by NHMRC 10 – 11 April 2003. National Health and Medical Research Council, Natural Resource Management Ministerial Council.

NZDWS, 2008: Drinking-water standards for New Zealand 2005 (Revised 2008). Ministry of Health, Wellington.

WHO, 2006: Guidelines for Drinking-water Quality 2006.

IARC, 2009: IARC Monographs on the Evaluation of Carcinogenic Risks to Humans. International Agency for Research on Cancer. World Health Organisation. Classification: Group 1: Carcinogenic to humans; Group 2A: Probably carcinogenic to humans; Group 2B: Possibly carcinogenic to humans; Group 3: Not classifiable as to carcinogenicity to humans; Group 4: Probably not carcinogenic to humans.

ECOTOX, US Environmental Protection Agency ECOTOX database contained over 500 test results, data selected as LC50 and NOEC from common species used for toxicity testing with non-physiological end points; data presented as ¹geometric mean (range) N=3; ²geometric mean (range) N=11; ³geometric mean (range) N=5; ⁴geometric mean (range) N=7.

ECOSAR, US Environmental Protection Agency ECOSAR database , Ecological Structure Activity Relationships (ECOSAR) Class Program. Accessed at <http://www.epa.gov/oppt/newchems/tools/21ecosar.htm>.



Name	5-chloro-2-methyl-4-isothiazolin-3-one
Synonyms	Methylchloroisothiazolinone
CAS number	26172-55-4
Molecular formula	C ₄ H ₄ CINOS
Product name	M275

Physical Properties	Value	Reference
Phase/state	NA	
Molecular weight	149.60 g/mol	EPI SUITE
Melting point	50-55°C	IUCLID, 2000
Boiling point	106.5 °C	IUCLID, 2000
Density/ specific gravity	1.2556 g/m ³ at 20 °C	IUCLID, 2000
Vapour pressure	20.8 hPa at 20°C	IUCLID, 2000
Solubility	>5000 mg/l at 20 °C	IUCLID, 2000
	1.487 x 10 ⁵ mg/L at 25°C	EPI SUITE
Henrys law constant	3.57 x 10 ⁻⁸ atm-m ³ /mol at 25°C (Bond method)	EPI SUITE
Organic carbon partition coefficient (Koc)	19.38 (MCI Method)	EPI SUITE
Log organic carbon partition coefficient (log Koc)	1.287 (MCI Method)	EPI SUITE
Log octanol-water partition coefficient (log Kow)	-0.34	EPI SUITE

Persistence/ Bioaccumulation	Value	Reference
Aquatic biodegradation	NA	
Aerobic BOD	97% after 48 hours	IUCLID, 2000
Anaerobic BOD	NA	
Biowin7 (Anerobic linear model)	Biodegrades fast	EPI SUITE
Fugacity		
Air %	0.251	EPI SUITE
Water %	32.4	EPI SUITE
Soil %	67.2	EPI SUITE
Sediment %	0.0918	EPI SUITE
Bioconcentration factor	3.162 L/kg wet wt	EPI SUITE
Biotransformation half-life	0.04781 days	EPI SUITE

- Notes: 1 EPI Suite™ v4.0, United States Environmental Protection Agency.
 2. Schluberger. Material Safety Data Sheet M275. Issue Date:16 July 2003.
 3. International Uniform Chemical Information database, 2000 (IUCLID). European Chemical Substances Information System Accessed online 14 April 2011 <http://ecb.jrc.ec.europa.eu/iuclid-datasheet/26172554.pdf>.
 NA - not available

Chemical Information Sheet - 5-chloro-2-methyl-4-isothiazolin-3-one

Chemical Information Sheet updated June 2011.

Aquatic toxicity guidelines				
Guideline	Year	Type	Value (g/m ³)	Notes
ANZECC	2000	Aquatic toxicity	NA	
USEPA	2006	Aquatic toxicity	NA	
Other water quality guidelines				
Guideline	Year	Type	Value (g/m ³)	Notes
ADWG	2004	Drinking water	NA	
NZDWS	2008	Drinking water	NA	
WHO	2006	Drinking water	NA	
USEPA	2006	Human Health	NA	
IARC	2006	Carcinogen risk	NA	
ANZECC	2000	Stock water	NA	

Aquatic Ecotoxicological Data

Acute toxicity data							
Species name	Common name	Endpoint	Effect	Effect measure	Test time (days)	Conc (µg/L)	Reference
Oncorhynchus mykiss	Rainbow Trout	LC50	MOR	MORT	14	80	ECOTOX
Daphnia magna	Water Flea	EC50	ITX	IMBL	2	180	ECOTOX
Oncorhynchus mykiss	Rainbow Trout	LC50	MOR	MORT	4	190	ECOTOX
Oncorhynchus mykiss	Rainbow Trout	LC50	MOR	MORT	4	253	ECOTOX
Lepomis macrochirus	Bluegill	LC50	MOR	MORT	4	300	ECOTOX
Daphnia magna	Water Flea	EC50	ITX	IMBL	2	840	ECOTOX
Lepomis macrochirus	Bluegill	LC50	MOR	MORT	4	960	ECOTOX
Daphnia magna	Water Flea	EC50	ITX	IMBL	2	1300	ECOTOX
Oncorhynchus mykiss	Rainbow Trout	LC50	MOR	MORT	4	1520	ECOTOX
Lepomis macrochirus	Bluegill	LC50	MOR	MORT	4	2130	ECOTOX
Ceriodaphnia dubia	Water Flea	EC50	ITX	IMBL	2	13000	ECOTOX
Chronic toxicity data							
Pseudokirchneriella subcapitata	Green Algae	EC50	POP	ABND	5	22	ECOTOX
Pseudokirchneriella subcapitata	Green Algae	EC50	POP	ABND	4	62	ECOTOX
Pseudokirchneriella subcapitata	Green Algae	EC50	POP	ABND	3	130	ECOTOX
Anabaena flosaquae	Blue-Green Algae	EC50	POP	ABND	5	290	ECOTOX
Lemna gibba	Inflated Duckweed	EC50	POP	ABND	14	4500	ECOTOX

Media Type : Freshwater

ITX : Intoxication

IMBL: Immobile

MOR / MORT: Mortality

POP: Population

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Chemical Information Sheet - 5-chloro-2-methyl-4-isothiazolin-3-one

ABND : Abundance

Notes: ANZECC, 2000: Australian and New Zealand guidelines for fresh and marine water quality. Australian and New Zealand Environment and Conservation Council.

USEPA, 2006: National recommended water quality criteria: 2006. EPA-822-R-02-047. Office of Water and Office of Science and Technology, United States Environmental Protection Agency.

ADWG, 2004: Australian drinking water guidelines . Endorsed by NHMRC 10 – 11 April 2003. National Health and Medical Research Council, Natural Resource Management Ministerial Council.

NZDWS, 2008: Drinking-water standards for New Zealand 2005 (Revised 2008). Ministry of Health, Wellington.

WHO, 2006: Guidelines for Drinking-water Quality 2006.

IARC, 2009: IARC Monographs on the Evaluation of Carcinogenic Risks to Humans. International Agency for Research on Cancer. World Health Organisation. Classification: Group 1: Carcinogenic to humans; Group 2A: Probably carcinogenic to humans; Group 2B: Possibly carcinogenic to humans; Group 3: Not classifiable as to carcinogenicity to humans; Group 4: Probably not carcinogenic to humans.

ECOTOX, US Environmental Protection Agency ECOTOX database contained over 500 test results, data selected as LC50 and NOEC from common species used for toxicity testing with non-physiological end points; data presented as ¹ geometric mean (range) N=3; ² geometric mean (range) N=11; ³ geometric mean (range) N=5; ⁴ geometric mean (range) N=7.

ECOSAR, US Environmental Protection Agency ECOSAR database , Ecological Structure Activity Relationships (ECOSAR) Class Program. Accessed at <http://www.epa.gov/oppt/newchems/tools/21ecosar.htm>.



Name	Tetrasodium ethylenediaminetetraacetate
Synonyms	Tetrasodium ethylenediaminetetraacetate, Tetrasodium EDTA, Acetic Acid, N,N'-1,2-EthanediyI bis[N-(carboxymethyl)glycine, sodium salt
CAS number	64-02-8
Molecular formula	C ₁₀ H ₁₆ N ₂ O ₈ Na ₄
Product name	Not specified

Physical Properties	Value	Reference
Phase/state	White powder	HSDB, 2011
Molecular weight	380.17 g/mol	HSDB, 2011
Melting point	>300 °C	HSDB, 2011
Boiling point	572.7 °C (estimate)	EPISUITE
Density/ specific gravity	6.9 lb/gal apparent density	HSDB 2011
Vapour pressure	1.49 x 10 ⁻¹² mm Hg at 25 °C	EPISUITE
Solubility	500 g/L at 20 °C in water 1 x 10 ⁶ at 25 °C in water	HSDB, 2011 EPISUITE
Henrys law constant	1.18x10 ⁻²³ atm m ³ /mol	HSDB, 2011
Organic carbon partition coefficient (Koc)	312.7	EPISUITE
Log organic carbon partition coefficient (log Koc)	2.495	EPISUITE
Log octanol-water partition coefficient (log Kow)	-13.17*	EPISUITE

*This molar concentration is not possible but results from the extreme Log Kow value predicted by EPISUITE. It has not been relied upon. A measured value for Kow for this compound could not be found.

Persistence/ Bioaccumulation	Value	Reference
Aquatic biodegradation	NA	
Aerobic BOD	NA	
Anaerobic BOD	NA	
Biowin7 (Anaerobic Model Prediction)	Biodegrades fast	EPISUITE
Fugacity		
Air %	1.36 x 10 ⁻¹²	EPISUITE
Water %	18.9	EPISUITE
Soil %	80.9	EPISUITE
Sediment %	0.198	EPISUITE
Bioconcentration factor (BCF)	3.162	EPISUITE
Biotransformation half-life	7.617x 10 ⁻⁶	EPISUITE

Notes: 1 EPI Suite™ v4.1, United States Environmental Protection Agency.

2. Hazardous Substances Data Bank (HSDB) National library of Medicine accessed on line: 25 March 2011.

NA - not available

Aquatic toxicity guidelines				
Guideline	Year	Type	Value (g/m ³)	Notes
ANZECC	2000	Aquatic toxicity	NA	
USEPA	2006	Aquatic toxicity	NA	
Other water quality guidelines				
Guideline	Year	Type	Value (g/m ³)	Notes
ADWG	2004	Drinking water	NA	
NZDWS	2008	Drinking water	NA	
WHO	2006	Drinking water	NA	
USEPA	2006	Human Health	NA	
IARC	2006	Carcinogen risk	NA	
ANZECC	2000	Stock water	NA	

Aquatic Toxicological Data

Acute toxicity data							
Species Name	Common Name	Endpoint	Effect	Effect Measure	Test Time (Days)	Conc (µg/L)	Reference
Lepomis macrochirus	Bluegill	LC50	MOR	MORT	4	486000	ECOTOX
Daphnia magna	Water Flea	EC50	MOR	MORT	1	610000	ECOTOX
Lepomis macrochirus	Bluegill	LC50	MOR	MORT	4	1030000	ECOTOX
Lepomis macrochirus	Bluegill	LC50	MOR	MORT	4	2070000	ECOTOX
Lepomis macrochirus	Bluegill	LC50	MOR	MORT	4	3092000	ECOTOX

Media Type: freshwater

IMBL: immobile

ABND: abundance

ITX : Intoxicated

MOR/MORT: Mortality

POP: Population

REP: Reproduction

PROG : Progeny Counts

SEXR : Sex ratio

FCND: Fecundity

HTCH : Hatch

Notes: ANZECC, 2000: Australian and New Zealand guidelines for fresh and marine water quality. Australian and New Zealand Environment and Conservation Council.

USEPA, 2006: National recommended water quality criteria: 2006. EPA-822-R-02-047. Office of Water and Office of Science and Technology, United States Environmental Protection Agency.

ADWG, 2004: Australian drinking water guidelines . Endorsed by NHMRC 10 – 11 April 2003. National Health and Medical Research Council, Natural Resource Management Ministerial Council.

NZDWS, 2008: Drinking-water standards for New Zealand 2005 (Revised 2008). Ministry of Health, Wellington.

WHO, 2006: Guidelines for Drinking-water Quality 2006.

IARC, 2009: IARC Monographs on the Evaluation of Carcinogenic Risks to Humans. International Agency for Research on Cancer. World Health Organisation. Classification: Group 1: Carcinogenic to humans; Group 2A: Probably carcinogenic to humans; Group 2B: Possibly carcinogenic to humans; Group 3: Not classifiable as to carcinogenicity to humans; Group 4: Probably not carcinogenic to humans.

Chemical Information Sheet - Terasodium ethylenediaminetetraacetate

ECOTOX, US Environmental Protection Agency ECOTOX database contained over 500 test results, data selected as LC50 and NOEC from common species used for toxicity testing with non-physiological end points; data presented as ¹ geometric mean (range) N=3; ² geometric mean (range) N=11; ³ geometric mean (range) N=5; ⁴ geometric mean (range) N=7.
ECOSAR, US Environmental Protection Agency ECOSAR database , Ecological Structure Activity Relationships (ECOSAR) Class Program. Accessed at <http://www.epa.gov/oppt/newchems/tools/21ecosar.htm>.



Name	Vinylidene Chloride / Methylacrylate
Synonyms	1,1 dichloroethene, 1,1 dichloroethylene, 1,1 DCE, vinylidene dichloride.
CAS number	25038-72-6 (surrogate CAS 75-35-4 (1,1 DCE) used for the information on the chemical information sheet).
Molecular formula	C ₂ H ₂ Cl ₂
Product name	Not specified

Physical Properties	Value	Reference
Phase/state	Colourless liquid	HSDB, 2011
Molecular weight	96.94 g/mol	HSDB, 2011
Melting point	-122.5 °C	HSDB, 2011
Boiling point	31.7 °C	HSDB, 2011
Density/ specific gravity	1.2129 at 20°C	HSDB, 2011
Vapour pressure	600 mm Hg at 25°C	HSDB, 2011
Solubility	2,420 mg/L at 25°C	HSDB, 2011
Henry's law constant	2.61 x 10 ⁻² atm cu m/mole at 24 °C	HSDB, 2011
Organic carbon partition coefficient (K _{oc})	64	HSDB, 2011
Log organic carbon partition coefficient (log K _{oc})	1.80618	HSDB, 2011
Log octanol-water partition coefficient (log K _{ow})	2.12	EPISUITE

Persistence/ Bioaccumulation	Value	Reference
Aquatic biodegradation	Biodegradation in water is not expected to be an important fate process, with 1,1-DCE reaching 0% of its theoretical BOD in 4 weeks(11).	HSDB, 2011
Aerobic BOD	1,1-DCE had a biodegradation half-life of 1.25 yrs in ground water from a former manufacturing facility.	HSDB, 2011
Anaerobic BOD	In the microcosms designed to simulate a groundwater environment, 50% of the 1,1-dichloroethylene disappeared in 5-6 months	HSDB, 2011
Biowin7 (Anaerobic Model Prediction)	Does not biodegrades fast	EPISUITE
Fugacity		
Air %	20.8	EPISUITE
Water %	75.1	EPISUITE
Soil %	3.8	EPISUITE
Sediment %	0.257	EPISUITE
Bioconcentration factor (BCF)	11.81	EPISUITE
Biotransformation half-life	0.614 days	EPISUITE

Notes: 1 EPI Suite™ v4.0, United States Environmental Protection Agency.

Chemical Information Sheet - Vinylidene Chloride

2. Hazardous Substances Data Bank (HSDB) National library of Medicine accessed on line: 04 July 2011.

NA - not available

Aquatic toxicity guidelines				
Guideline	Year	Type	Value (g/m ³)	Notes
ANZECC	2000	Aquatic toxicity	NA	
USEPA	2006	Aquatic toxicity	0.38 ug/L	Human consumption of surface water
Other water quality guidelines				
Guideline	Year	Type	Value (g/m ³)	Notes
ADWG	2004	Drinking water	0.03 mg/L	Health guideline value
NZDWS	2008	Drinking water	NA	
WHO	2006	Drinking water	0.03 mg/L	
USEPA	2010	Human Health	2.4 x 10 ² mg/kg	
IARC	2006	Carcinogen risk	3	Not classifiable as to its carcinogenicity to humans
ANZECC	2000	Stock water	NA	

Surrogate 1,1 DCE 75-35-4 used for aquatic toxicity guidelines.

Aquatic Toxicological Data

Acute Toxicity Data							
Species Scientific Name	Species Common Name	Endpoint	Effect	Effect Measurement	Test time (days)	Conc 1 (ug/L)	Reference
Daphnia magna	Water Flea	LC50	MOR	MORT	1	11600	ECOTOX
Daphnia magna	Water Flea	LC50	MOR	MORT	2	11600	ECOTOX
Lepomis macrochirus	Bluegill	LC50	MOR	MORT	1	74000	ECOTOX
Lepomis macrochirus	Bluegill	LC50	MOR	MORT	4	74000	ECOTOX
Daphnia magna	Water Flea	LC50	MOR	MORT	2	79000	ECOTOX
Daphnia magna	Water Flea	LC50	MOR	MORT	1	98000	ECOTOX
Pimephales promelas	Fathead Minnow	LC50	MOR	MORT	2	108000	ECOTOX
Pimephales promelas	Fathead Minnow	LC50	MOR	MORT	4	108000	ECOTOX
Pimephales promelas	Fathead Minnow	LC50	MOR	MORT	1	116000	ECOTOX
Pimephales promelas	Fathead Minnow	LC50	MOR	MORT	2	169000	ECOTOX
Pimephales promelas	Fathead Minnow	LC50	MOR	MORT	4	169000	ECOTOX
Pimephales promelas	Fathead Minnow	LC50	MOR	MORT	1	175000	ECOTOX
Lepomis macrochirus	Bluegill	LC50	MOR	MORT	4	220000	ECOTOX
Chronic Toxicity Data							
Species Scientific Name	Species Common Name	Endpoint	Effect	Effect Measurement	Test time (days)	Conc 1 (ug/L)	Reference
Chlamydomonas reinhardtii	Green Algae	EC50	POP	BMAS	3	9120	ECOTOX
Pimephales promelas	Fathead Minnow	LC50	MOR	MORT	7	29000	ECOTOX
Pimephales promelas	Fathead Minnow	LC50	MOR	MORT	8	29000	ECOTOX
Pimephales promelas	Fathead Minnow	LC50	MOR	MORT	9	29000	ECOTOX
Pimephales promelas	Fathead Minnow	LC50	MOR	MORT	10	29000	ECOTOX
Pimephales promelas	Fathead Minnow	LC50	MOR	MORT	11	29000	ECOTOX

Chemical Information Sheet - Vinylidene Chloride

Species Scientific Name	Species Common Name	Endpoint	Effect	Effect Measurement	Test time (days)	Conc 1 (ug/L)	Reference
Pimephales promelas	Fathead Minnow	LC50	MOR	MORT	12	29000	ECOTOX
Pimephales promelas	Fathead Minnow	LC50	MOR	MORT	13	29000	ECOTOX
Pimephales promelas	Fathead Minnow	LC50	MOR	MORT	6	74000	ECOTOX
Pimephales promelas	Fathead Minnow	LC50	MOR	MORT	5	97000	ECOTOX
Scenedesmus abundans	Green Algae	EC50	GRO	GGRO	4	410000	ECOTOX
Pseudokirchneriella subcapitata	Green Algae	EC50	POP	ABND	4	560000	ECOTOX

Media Type: freshwater

IMBL: immobile

ABND: abundance

ITX : Intoxicated

MOR/MORT: Mortality

POP: Population

REP: Reproduction

PROG : Progeny Counts

SEXR : Sex ratio

FCND: Fecundity

HTCH : Hatch

Notes: ANZECC, 2000: Australian and New Zealand guidelines for fresh and marine water quality. Australian and New Zealand Environment and Conservation Council.

USEPA, 2011: National recommended water quality criteria: 2011. United States Environmental Protection Agency. Accessed at : <http://water.epa.gov/scitech/swguidance/standards/current/index.cfm>

USEPA 2011: Regional Screening Level Table. United States Environmental Protection Agency Accessed at : http://www.epa.gov/reg3hwmd/risk/human/rb-concentration_table/Generic_Tables/pdf/master_sl_table_run_JUN2011.pdf

ADWG, 2004: Australian drinking water guidelines . Endorsed by NHMRC 10 – 11 April 2003. National Health and Medical Research Council, Natural Resource Management Ministerial Council.

NZDWS, 2008: Drinking-water standards for New Zealand 2005 (Revised 2008). Ministry of Health, Wellington.

WHO, 2006: Guidelines for Drinking-water Quality 2006.

IARC, 2009: IARC Monographs on the Evaluation of Carcinogenic Risks to Humans. International Agency for Research on Cancer. World Health Organisation. Classification: Group 1: Carcinogenic to humans; Group 2A: Probably carcinogenic to humans; Group 2B: Possibly carcinogenic to humans; Group 3: Not classifiable as to carcinogenicity to humans; Group 4: Probably not carcinogenic to humans.

ECOTOX, US Environmental Protection Agency ECOTOX database contained over 500 test results, data selected as LC50 and NOEC from common species used for toxicity testing with non-physiological end points; data presented as ¹ geometric mean (range) N=3; ² geometric mean (range) N=11; ³ geometric mean (range) N=5; ⁴ geometric mean (range) N=7.

ECOSAR, US Environmental Protection Agency ECOSAR database , Ecological Structure Activity Relationships (ECOSAR) Class Program. Accessed at <http://www.epa.gov/oppt/newchems/tools/21ecosar.htm>.



Name	1,2-benzisothiazolin-3-one
Synonyms	1,2 benzisothiazol 3 (2H) one, proxel PL
CAS number	2634-33-5
Molecular formula	C ₇ H ₅ NOS
Product name	

Physical Properties	Value	Reference
Phase/state	Solid, faintly yellow, forms crystals	Sigma-Aldrich 2007
Molecular weight	151.2 g/mol	Sigma-Aldrich 2007
Melting point	121.6°C (estimate)	EPISUITE
Boiling point	339.5 °C (estimate)	EPISUITE
Density/ specific gravity	NA	
Vapour pressure	2.57 x 10 ⁻⁵ mm Hg at 25°C (estimate)	EPISUITE
Solubility	2.143 x 10 ⁴ mg/L at 25°C (estimate)	EPISUITE
Henrys law constant	6.92 x 10 ⁻⁹ atm m ³ /mol (estimate)	EPISUITE
Organic carbon partition coefficient (Koc)	34.48 (MCI Method (estimate))	EPISUITE
Log organic carbon partition coefficient (log Koc)	1.538 (MCI Method) (estimate)	EPISUITE
Log octanol-water partition coefficient (log Kow)	0.64 (estimate)	EPISUITE

Persistence/ Bioaccumulation	Value	Reference
Aquatic biodegradation	NA	
Aerobic BOD	NA	
Anaerobic BOD	NA	
Biowin7 (Anaerobic Model Prediction)	Does not biodegrade fast	EPISUITE
Fugacity		
Air %	0.129 (estimate)	EPISUITE
Water %	24.4 (estimate)	EPISUITE
Soil %	75.4 (estimate)	EPISUITE
Sediment %	0.0796 (estimate)	EPISUITE
Bioconcentration factor (BCF)	3.162 L/kg wet wt (estimate)	EPISUITE
Biotransformation half-life	0.2548 days (estimate)	EPISUITE

Notes: 1 EPI Suite™ v4.0, United States Environmental Protection Agency.

2. Sigma Aldrich (2007). 1,2 benzisothiazolin 3 one Material Safety Data Sheet. Accessed on 7th June 2011. Accessed at : http://www.hopefortruth.com/LBAM_Forms/benisothiazol%20MSDS.pdf

NA - not available

Aquatic toxicity guidelines				
Guideline	Year	Type	Value (g/m ³)	Notes
ANZECC	2000	Aquatic toxicity	NA	
USEPA	2006	Aquatic toxicity	NA	

Chemical Information Sheet - 1,2 benzisothiazolin 3 one

Other water quality guidelines				
Guideline	Year	Type	Value (g/m ³)	Notes
ADWG	2004	Drinking water	NA	
NZDWS	2008	Drinking water	NA	
WHO	2006	Drinking water	NA	
USEPA	2006	Human Health	NA	
IARC	2006	Carcinogen risk	NA	
ANZECC	2000	Stock water	NA	

Aquatic Toxicological Data

Acute toxicity data							
Species Name	Common Name	Endpoint	Effect	Effect Measure	Test Time (Days)	Conc (µg/L)	Reference
Oncorhynchus mykiss	Rainbow Trout	LC50	MOR	MORT	4	1600	ECOTOX
Daphnia magna	Water Flea	EC50	ITX	IMBL	2	4400	ECOTOX

Media Type: freshwater

IMBL: immobile

ABND: abundance

ITX : Intoxicated

MOR/MORT: Mortality

POP: Population

REP: Reproduction

PROG : Progeny Counts

SEXR : Sex ratio

FCND: Fecundity

HTCH : Hatch

Notes: ANZECC, 2000: Australian and New Zealand guidelines for fresh and marine water quality. Australian and New Zealand Environment and Conservation Council.

USEPA, 2006: National recommended water quality criteria: 2006. EPA-822-R-02-047. Office of Water and Office of Science and Technology, United States Environmental Protection Agency.

ADWG, 2004: Australian drinking water guidelines . Endorsed by NHMRC 10 – 11 April 2003. National Health and Medical Research Council, Natural Resource Management Ministerial Council.

NZDWS, 2008: Drinking-water standards for New Zealand 2005 (Revised 2008). Ministry of Health, Wellington.

WHO, 2006: Guidelines for Drinking-water Quality 2006.

IARC, 2009: IARC Monographs on the Evaluation of Carcinogenic Risks to Humans. International Agency for Research on Cancer. World Health Organisation. Classification: Group 1: Carcinogenic to humans; Group 2A: Probably carcinogenic to humans; Group 2B: Possibly carcinogenic to humans; Group 3: Not classifiable as to carcinogenicity to humans; Group 4: Probably not carcinogenic to humans.

ECOTOX, US Environmental Protection Agency ECOTOX database contained over 500 test results, data selected as LC50 and NOEC from common species used for toxicity testing with non-physiological end points; data presented as ¹ geometric mean (range) N=3; ² geometric mean (range) N=11; ³ geometric mean (range) N=5; ⁴ geometric mean (range) N=7.

ECOSAR, US Environmental Protection Agency ECOSAR database , Ecological Structure Activity Relationships (ECOSAR) Class Program. Accessed at <http://www.epa.gov/oppt/newchems/tools/21ecosar.htm>.



Name	Sweet Orange Oil
Synonyms	Orange oil (composition of orange oil differs from sweet orange oil; its aldehyde content is lower and its ester content higher).
CAS number	68647-72-3 or 8008-57-9
Molecular formula	C10H16
Product name	GasPerm 1100

Physical Properties	Value	Reference
Phase/state	Yellow to reddish yellow liquid.	HSDB, 2011
Molecular weight	136.24	EPISUITE
Melting point	-40.76	EPISUITE
Boiling point	176 °C	Chembook 2011
Density/ specific gravity	0.844 - 0.847 at 20 °C	HSDB, 2011
Vapour pressure	NA	HSDB, 2011
Solubility	Slightly soluble in water	HSDB, 2011
	4.581 mg/L at 25 °C	EPISUITE
Henry's law constant	3.8×10^{-1} atm·m ³ / mol (Bond Method)	EPISUITE
Log organic carbon partition coefficient (log Koc)	3.049 (MCI Method)	EPISUITE
Log octanol-water partition coefficient (log Kow)	4.83	EPISUITE

Persistence/ Bioaccumulation	Value	Reference
Aquatic biodegradation	NA	HSDB, 2011
Aerobic BOD	NA	HSDB, 2011
Anaerobic BOD	NA	HSDB, 2011
Biowin7 (Anaerobic Model Prediction)	Does not biograde fast	EPISUITE
Fugacity		
Air %	0.298	EPISUITE
Water %	50.2	EPISUITE
Soil %	47.5	EPISUITE
Sediment %	1.96	EPISUITE
Bioconcentration factor (BCF)	360.5	EPISUITE
Biotransformation half-life	3.531 days	EPISUITE

- Notes: 1 EPI Suite™ v4.0, United States Environmental Protection Agency.
 2. Halliburton Material Safety Data Sheet GasPerm 1100. Issue Date: 4 March 2010.
 3. Hazardous Substances Data Bank (HSDB) National library of Medicine accessed on line: 25 March 201.
 NA - not available

Chemical Information Sheet - Sweet Orange Oil

Aquatic toxicity guidelines				
Guideline	Year	Type	Value (g/m ³)	Notes
ANZECC	2000	Aquatic toxicity	NA	
USEPA	2006	Aquatic toxicity	NA	
Other water quality guidelines				
Guideline	Year	Type	Value (g/m ³)	Notes
ADWG	2004	Drinking water	NA	
NZDWS	2008	Drinking water	NA	
WHO	2006	Drinking water	NA	
USEPA	2006	Human Health	NA	
IARC	2006	Carcinogen risk	NA	
ANZECC	2000	Stock water	NA	

Aquatic Toxicological Data

Estimated acute toxicity data							
Species name	Common name	Endpoint	Effect	Effect measure	Test time (days)	Concentration (ug/L)	Reference
-	Daphnid	LC50	MOR	MORT	2	292	ECOSAR v1.0
-	Fish	LC50	MOR	MORT	4	341	ECOSAR v1.0
-	Fish	LC50	MOR	MORT	14	361	ECOSAR v1.0
Estimated chronic toxicity data							
-	Green Algae	EC50	POP	GPOP	4	474	ECOSAR v1.0

Media Type : freshwater

MOR/MORT : Mortality

POP: Population

GPOP: Population changes, general

Notes: ANZECC, 2000: Australian and New Zealand guidelines for fresh and marine water quality. Australian and New Zealand Environment and Conservation Council.

USEPA, 2006: National recommended water quality criteria: 2006. EPA-822-R-02-047. Office of Water and Office of Science and Technology, United States Environmental Protection Agency.

ADWG, 2004: Australian drinking water guidelines . Endorsed by NHMRC 10 – 11 April 2003. National Health and Medical Research Council, Natural Resource Management Ministerial Council.

NZDWS, 2008: Drinking-water standards for New Zealand 2005 (Revised 2008). Ministry of Health, Wellington.

WHO, 2006: Guidelines for Drinking-water Quality 2006.

IARC, 2009: IARC Monographs on the Evaluation of Carcinogenic Risks to Humans. International Agency for Research on Cancer. World Health Organisation. Classification: Group 1: Carcinogenic to humans; Group 2A: Probably carcinogenic to humans; Group 2B: Possibly carcinogenic to humans; Group 3: Not classifiable as to carcinogenicity to humans; Group 4: Probably not carcinogenic to humans.

ECOTOX, US Environmental Protection Agency ECOTOX database contained over 500 test results, data selected as LC50 and NOEC from common species used for toxicity testing with non-physiological end points; data presented as ¹ geometric mean (range) N=3; ² geometric mean (range) N=11; ³ geometric mean (range) N=5; ⁴ geometric mean (range) N=7.

ECOSAR, US Environmental Protection Agency ECOSAR database , Ecological Structure Activity Relationships (ECOSAR) Class Program. Accessed at <http://www.epa.gov/oppt/newchems/tools/21ecosar.htm>.



Name	Fatty acid ester *
Synonyms	NA *
CAS number	NA *
Molecular formula	NA *
Product name	-

* Chemical name and identifiers not included due to commercial confidentiality. Refer to Table D3, Appendix D, for further details.

Physical Properties	Value	Reference
Phase/state	Amber liquid	HSDB 2011
Molecular weight	428.61	HSDB 2011
Melting point	0-10 °C	IUCLID 2000
Boiling point	>240 °C	IUCLID 2000
Density/ specific gravity	1 g/cm ³ at 20 °C	IUCLID 2000
Vapour pressure		
Solubility	Dispersible in water <10 g/L at 20 °C 0.01914 mg/L at 25 °C	HSDB 2011 IUCLID 2000 EPISUITE
Henry's law constant	1.42 x 10 ⁻¹² atm m ³ /mole (BOND Method)	EPISUITE
Organic carbon partition coefficient (K _{oc})	2423	EPISUITE
Log organic carbon partition coefficient (log K _{oc})	3.384	EPISUITE
Log octanol-water partition coefficient (log K _{ow})	5.89	EPISUITE

Persistence/ Bioaccumulation		Reference
Aquatic biodegradation		
Aerobic BOD		
Anaerobic BOD		
Ready Biodegradability Prediction	Readily biodegradable	EPISUITE
Fugacity		
Air %	0.101	EPISUITE
Water %	23.7	EPISUITE
Soil %	74.4	EPISUITE
Sediment %	1.78	EPISUITE
Bioconcentration factor (BCF)	149.9 L/kg wet-wt	EPISUITE
Biotransformation half-life	0.09698	EPISUITE

Notes: 1 EPI Suite™ v4.1, United States Environmental Protection Agency.

2. Hazardous Substances Data Bank (HSDB) National library of Medicine accessed on line 26/07/11

NA - not available

Chemical Information Sheet - Fatty Acid Ester

Aquatic toxicity guidelines				
Guideline	Year	Type	Value (mg/L)	Notes
ANZECC	2000	Aquatic toxicity	NA	
USEPA	2010	Aquatic toxicity	NA	
Other water quality guidelines				
Guideline	Year	Type	Value (mg/L)	Notes
ADWG	2004	Drinking water	NA	
NZDWS	2008	Drinking water	NA	
WHO	2006	Drinking water	NA	
USEPA	2010	Human Health	NA	
IARC	2006	Carcinogen risk	NA	
ANZECC	2000	Stock water	NA	

Aquatic Toxicological Data

Acute toxicity data							
Species Name	Common Name	Endpoint	Effect	Effect Measure	Test Time (Days)	Concentration (µg/L)	Reference
-	Daphnid	LC50	MOR	MORT	2	4.36E+02 ¹	ECOSAR v1.00
-	Daphnid	LC50	MOR	MORT	2	1.57E+02 ²	ECOSAR v1.00
-	Fish	LC50	MOR	MORT	4	3.50E+02 ¹	ECOSAR v1.00
-	Fish	LC50	MOR	MORT	4	1.70E+02 ²	ECOSAR v1.00
-	Daphnid	LC50	MOR	MORT	2	4.36E+02 ¹	ECOSAR v1.00

Chronic toxicity data							
Species Name	Common Name	Endpoint	Effect	Effect Measure	Test Time (Days)	Concentration (µg/L)	Reference
-	Green Algae	EC50	POP	GPOP	4	1.22E+02 ¹	ECOSAR v1.00
-	Green Algae	EC50	POP	GPOP	4	3.34E+02 ²	ECOSAR v1.00
-	Fish	EC50	MOR	MORT	14	1.49E+02 ¹	ECOSAR v1.00

¹Modelled as an ester

²Modelled as a neutral organic

MOR/MORT: Mortality

ITX/IMBL : Intoxication/Immobile

POP: Population

REP: Reproduction

GPOP: Population growth, general

ABND: Abundance

PGRT: Population growth rate

SPGR: Growth/specific growth rate

Notes: ANZECC, 2000: Australian and New Zealand guidelines for fresh and marine water quality. Australian and New Zealand Environment and Conservation Council.

Chemical Information Sheet - Fatty Acid Ester

USEPA, 2006: National recommended water quality criteria: 2006. EPA-822-R-02-047. Office of Water and Office of Science and Technology, United States Environmental Protection Agency.

ADWG, 2004: Australian drinking water guidelines . Endorsed by NHMRC 10 – 11 April 2003. National Health and Medical Research Council, Natural Resource Management Ministerial Council.

NZDWS, 2008: Drinking-water standards for New Zealand 2005 (Revised 2008). Ministry of Health, Wellington.

WHO, 2006: Guidelines for Drinking-water Quality 2006.

IARC, 2009: IARC Monographs on the Evaluation of Carcinogenic Risks to Humans. International Agency for Research on Cancer. World Health Organisation. Classification: Group 1: Carcinogenic to humans; Group 2A: Probably carcinogenic to humans; Group 2B: Possibly carcinogenic to humans; Group 3: Not classifiable as to carcinogenicity to humans; Group 4: Probably not carcinogenic to humans .

ECOTOX, United States Environmental Protection Agency ECOTOX database contained over 400 test, data selected as LC50 and NOEC from common species used for toxicity testing with non-physiological end points; and¹ data presented as geometric mean (range) N=8.

AJE, 1999: Organic Chemical Toxicity Data Database. Australasian Journal of Ecotoxicology. 5: 21-84.

RIVM, 2005. Environmental Risk Limit for Alcohols, glycols, and some other relatively soluble and /or volatile compounds. 1 ecotoxicological evaluation. RIVM report 601501016/2005

Name	Ethoxylated fatty acid ester *
Synonyms	NA *
CAS number	NA *
Molecular formula	NA *
Product name	-

* Chemical name and identifiers not included due to commercial confidentiality. Refer to Table D3, Appendix D, for further details.

Physical Properties	Value	Reference
Phase/state	Yellow to orange coloured oily liquid	HSDB 2011
Molecular weight	54	EPISUITE
Melting point	349.84 °C (estimate)	EPISUITE
Boiling point	1074.99 °C (estimate)	EPISUITE
Density/ specific gravity	1.06-1.10	HSDB 2011
Vapour pressure	NA	
Solubility	1.9 x 10 ⁻² mg/L at 25°C 0.01999 mg/L at 25°C	HSDB 2011 EPISUITE
Henry's law constant	1.05 x 10 ⁻³⁹	EPISUITE
Organic carbon partition coefficient (K _{oc})	8.78 x 10 ⁹ ^a	EPISUITE
Log organic carbon partition coefficient (log K _{oc})	9.943	EPISUITE
Log octanol-water partition coefficient (log K _{ow})	0.7	EPISUITE

Persistence/ Bioaccumulation		Reference
Aquatic biodegradation		
Aerobic BOD	1000 mg/L degraded by 17.8% over 20 days	HSDB 2011
Anaerobic BOD	200 mg/L exhibited 16.6% and 18.6% methane production in glucose and lactate fed cultures after 7 days.	HSDB 2011
Ready Biodegradability Prediction	Not readily bioadegradable	EPISUITE
Fugacity	3.12 x 10 ⁻⁸	EPISUITE
Air %	0.548	EPISUITE
Water %	52.1	EPISUITE
Soil %	47.4	EPISUITE
Sediment %		
Bioconcentration factor (BCF)	3.162 L/kg wet wt	EPISUITE
Biotransformation half-life	0.0002525 days	EPISUITE

Notes: 1. EPI Suite™ v4.1, United States Environmental Protection Agency.
2. Hazardous Substances Data Bank (HSDB) National library of Medicine accessed on line 26/07/11
NA - not available

^a EPISUITE provided two values for K_{oc}: 8.78 x 10⁹ L/kg using the MCI method and 0.6161 using the K_{ow} method. For consistency with other chemical sheets, the value derived using the MCI method has been included here.

Chemical Information Sheet - Ethoxylated Fatty Acid Ester

Aquatic toxicity guidelines				
Guideline	Year	Type	Value (mg/L)	Notes
ANZECC	2000	Aquatic toxicity	NA	
USEPA	2010	Aquatic toxicity	NA	
Other water quality guidelines				
Guideline	Year	Type	Value (mg/L)	Notes
ADWG	2004	Drinking water	NA	
NZDWS	2008	Drinking water	NA	
WHO	2006	Drinking water	NA	
USEPA	2010	Human Health	NA	
IARC	2006	Carcinogen risk	NA	
ANZECC	2000	Stock water	NA	

Aquatic Toxicological Data

Acute toxicity data							
Species Name	Common Name	Endpoint	Effect	Effect Measure	Test Time (Days)	Concentration (µg/L)	Reference
-	Daphnid	LC50	MOR	MORT	2	1.98E+06	ECOSAR v1.00
-	Fish	LC50	MOR	MORT	4	8.15E+05	ECOSAR v1.00

Chronic toxicity data							
Species Name	Common Name	Endpoint	Effect	Effect Measure	Test Time (Days)	Concentration (µg/L)	Reference
-	Green Algae	EC50	POP	GPOP	4	9.70E+05	ECOSAR v1.00
-	Fish	EC50	MOR	MORT	14	8.20E+08	ECOSAR v1.00

MOR/MORT: Mortality

ITX/IMBL : Intoxication/Immobile

POP: Population

REP: Reproduction

GPOP: Population growth, general

ABND: Abundance

PGRT: Population growth rate

SPGR: Growth/specific growth rate

Notes: ANZECC, 2000: Australian and New Zealand guidelines for fresh and marine water quality. Australian and New Zealand Environment and Conservation Council.

USEPA, 2006: National recommended water quality criteria: 2006. EPA-822-R-02-047. Office of Water and Office of Science and Technology, United States Environmental Protection Agency.

ADWG, 2004: Australian drinking water guidelines . Endorsed by NHMRC 10 – 11 April 2003. National Health and Medical Research Council, Natural Resource Management Ministerial Council.

NZDWS, 2008: Drinking-water standards for New Zealand 2005 (Revised 2008). Ministry of Health, Wellington.

Chemical Information Sheet - Ethoxylated Fatty Acid Ester

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IARC, 2009: IARC Monographs on the Evaluation of Carcinogenic Risks to Humans. International Agency for Research on Cancer. World Health Organisation. Classification: Group 1: Carcinogenic to humans; Group 2A: Probably carcinogenic to humans; Group 2B: Possibly carcinogenic to humans; Group 3: Not classifiable as to carcinogenicity to humans; Group 4: Probably not carcinogenic to humans .

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