2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) (CAS# 2224-33-1)
GreenScreen® for Safer Chemicals (GreenScreen®) Assessment

Prepared for:

Washington State Department of Ecology

Prepared by:

ToxServices LLC

October 17, 2014

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2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) is a chemical that is used as a cross-linking agent in room temperature vulcanizing silicone adhesive sealant. In general, 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) is used at a concentration less than 10% in these formulations. During the production of room temperature vulcanizing silicone adhesive sealants, 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) reacts with silanol polymers in the formulation during compounding and then further reacts during exposure to moisture. The parent silane is consumed into the polymer matrix and no longer exists after curing; therefore, consumer exposure to 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) is greatly reduced.

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) was assigned a GreenScreen® Benchmark Score of 1_{TP} ("Avoid-Chemical of High Concern") due to the transformation product methyl ethyl ketoxime (LT-1). 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) itself was assigned a GreenScreen® Benchmark score of 2 ("Use but Search for Safer Substitutes"-insufficient data to reach a higher Benchmark score) as it has High Group II* Human Toxicity (systemic toxicity repeated dose (STr*)). This corresponds to GreenScreen® benchmark classification 2f in CPA 2011. Data gaps (DG) exist for endocrine activity (E), respiratory sensitization (SnR*), and chronic aquatic toxicity (CA). As outlined in CPA (2013) Section 12.2 (Step 8 – Conduct a Data Gap Analysis to assign a final Benchmark score), 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne) trioxime) meets requirements for a GreenScreen® Benchmark Score of 2 despite the hazard data gaps. In a worst-case scenario, if 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne) trioxime) were assigned a High score for the data gap endocrine activity (E), it would be categorized as a Benchmark 1 Chemical.

GreenScreen® Benchmark Score for Relevant Route of Exposure:
As a standard approach for GreenScreen® evaluations, all exposure routes (oral, dermal, and inhalation) were evaluated together, so the GreenScreen® Benchmark Score of 1_{TP} ("Avoid-Chemical of High Concern") is applicable for all routes of exposure.

GreenScreen® Hazard Ratings for 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime)

Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
						single	repeated*	single	repeated*										
L	**L**	**L**	**L**	DG	**M**	**M**	*H*	**M**	**M**	**M**	DG	*M*	**H**	**M**	DG	**L**	**vL**	**L**	*M*

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect estimated values, authoritative B lists, screening lists, weak analogues, and lower confidence. Hazard levels in **BOLD** font are used with good quality data, authoritative A lists, or strong analogues. Group II Human Health endpoints differ from Group II* Human Health endpoints in that they have four hazard scores (i.e., vH, H, M, and L) instead of three (i.e., H, M, and L), and are based on single exposures instead of repeated exposures. Please see Appendix A for a glossary of hazard acronyms.

GreenScreen® Assessment for 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) (CAS #2224-33-1)

Method Version: GreenScreen® Version 1.2[1]
Assessment Type[2]: Certified

Chemical Name: 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime)

CAS Number: 2224-33-1

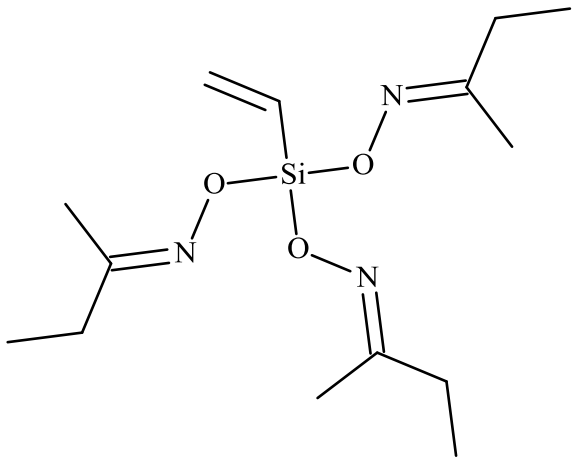
GreenScreen® Assessment Prepared By:
Name: Sara M. Ciotti, Ph.D.

Title: Toxicologist
Organization: ToxServices LLC
Date: October 8, 2014
Assessor Type: Licensed GreenScreen® Profiler

Quality Control Performed By:
Name: Dr. Margaret H. Whittaker, Ph.D., M.P.H., CBiol., F.S.B., E.R.T., D.A.B.T.
Title: Managing Director and Chief Toxicologist
Organization: ToxServices LLC
Date: October 17, 2014

Confirm application of the *de minimus* rule[3]: N/A

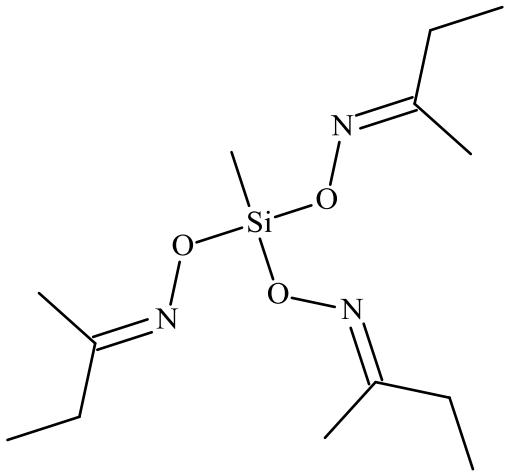
Chemical Structure(s):



Also called: 2-Butanone, O,O',O''-(ethenylsilylidyne)trioxime; Butan-2-one O,O',O''-(vinylsilylidyne)trioxime (ChemIDplus 2014)

[1] Use GreenScreen® Assessment Procedure (Guidance) V1.2
[2] GreenScreen® reports are either "UNACCREDITED" (by unaccredited person), "AUTHORIZED" (by Authorized GreenScreen® Practitioner), "CERTIFIED" (by Licensed GreenScreen® Profiler or equivalent) or "CERTIFIED WITH VERIFICATION" (Certified or Authorized assessment that has passed GreenScreen® Verification Program)
[3] Every chemical in a material or formulation should be assessed if it is:
1. intentionally added and/or
2. present at greater than or equal to 100 ppm

Chemical Structure(s) of Chemical Surrogates Used in the GreenScreen®:
2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) was assessed as a member of the oximino silanes category by UNEP (2009). The other member of the oximino silanes category, 2-butanone, O,O',O''-(methylsilylidyne)trioxime, was used as a surrogate in this GreenScreen®. 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) and 2-butanone, O,O',O''-(methylsilylidyne)trioxime both contain three methylethylketoxime groups and one methyl or vinyl in the fourth position on the silicon atom. Both substances hydrolyze very rapidly and they have similar physicochemical properties.



2-Butanone, O,O',O''-(methylsilylidyne)trioxime (CAS# 22984-54-9)

Identify Applications/Functional Uses: (UNEP 2009)
1. Cross-linking agent

<u>GreenScreen® Summary Rating for 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime)</u>[4]:
2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) was assigned a GreenScreen® Benchmark Score of 1_{TP} ("Avoid-Chemical of High Concern") due to the transformation product methyl ethyl ketoxime (LT-1). 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) itself was assigned a GreenScreen® Benchmark score of 2 ("Use but Search for Safer Substitutes"-insufficient data to reach a higher Benchmark score) as it has High Group II* Human Toxicity (systemic toxicity repeated dose (STr*)). This corresponds to GreenScreen® benchmark classification 2f in CPA 2011. Data gaps (DG) exist for endocrine activity (E), respiratory sensitization (SnR*), and chronic aquatic toxicity (CA). As outlined in CPA (2013) Section 12.2 (Step 8 – Conduct a Data Gap Analysis to assign a final Benchmark score), 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) meets requirements for a GreenScreen® Benchmark Score of 2 despite the hazard data gaps. In a worst-case scenario, if 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) were assigned a High score for the data gap endocrine activity (E), it would be categorized as a Benchmark 1 Chemical.

[4] For inorganic chemicals with low human and ecotoxicity across all hazard endpoints and low bioaccumulation potential, persistence alone will not be deemed problematic. Inorganic chemicals that are only persistent will be evaluated under the criteria for Benchmark 4.

Figure 1: GreenScreen® Hazard Ratings for 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime

Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
						single	repeated*	single	repeated*										
L	L	L	L	DG	M	M	*H*	M	M	M	DG	*M*	H	M	DG	L	vL	L	*M*

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect estimated (modeled) values, authoritative B lists, screening lists, weak analogues and lower confidence. Hazard levels in **BOLD** font are used with good quality data, authoritative A lists, or strong analogues. Group II Human Health endpoints differ from Group II* Human Health endpoints in that they have four hazard scores (i.e. vH, H, M, and L) instead of three (i.e. H, M, and L), and are based on single exposures instead of repeated exposures. Please see Appendix A for a glossary of hazard acronyms.

Transformation Products and Ratings:

Identify feasible and relevant fate and transformation products (i.e., dissociation products, transformation products, valence states) **and/or moieties of concern**[5]

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) undergoes rapid hydrolysis to form three moles of methyl ethyl ketoxime (CAS# 96-29-7) and one mole of reactive vinyl substituted silanetriol. If vinyl substituted silanetriol is present at a concentration greater than 500 mg/L it can condense to form substituted silanes (UNEP 2009). As the transformation product methyl ethyl ketoxime is an LT-1, the benchmark score of 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) was adjusted.

Functional Use	Life Cycle Stage	Transformation Pathway	Transformation Products	CAS #	Feasible and Relevant?	GreenScreen® List Translator Score or Benchmark Score[6,7]
N/A	N/A	Hydrolysis	Methyl ethyl ketoxime	96-29-7	Yes	LT-1 (MAK: Carcinogen Group 2)

Introduction

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) is a chemical that is used as a cross-linking agent in room temperature vulcanizing silicone adhesive sealant. In general 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) is used at a concentration less than 10% in these formulations. During the production of room temperature vulcanizing silicone adhesive sealants, 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) reacts with silanol polymers in the formulation during compounding and then further reacts during exposure to moisture. The parent silane is consumed into

[5] A moiety is a discrete chemical entity that is a constituent part or component of a substance. A moiety of concern is often the parent substance itself for organic compounds. For inorganic compounds, the moiety of concern is typically a dissociated component of the substance or a transformation product.
[6] The GreenScreen® List Translator identifies specific authoritative or screening lists that should be searched to screen for GreenScreen® benchmark 1 chemicals (CPA 2012b). Pharos (Pharos 2014) is an online list-searching tool that is used to screen chemicals against the lists in the List Translator electronically.
[7] The way you conduct assessments for transformation products depends on the Benchmark Score of the parent chemical (See Guidance).

the polymer matrix and no longer exists after curing; therefore, consumer exposure to 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) is greatly reduced (UNEP 2009).

ToxServices assessed 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime against GreenScreen® Version 1.2 (CPA 2013) following procedures outlined in ToxServices' SOP 1.69 (GreenScreen® Hazard Assessment) (ToxServices 2013).

GreenScreen® List Translator Screening Results

The GreenScreen® List Translator identifies specific authoritative or screening lists that should be searched to identify GreenScreen® benchmark 1 chemicals (CPA 2012b). Pharos (Pharos 2014) is an online list-searching tool that is used to screen chemicals against the List Translator electronically. It checks all of the lists in the List Translator with the exception of the U.S. Department of Transportation (U.S. DOT) lists (U.S. DOT 2008a,b) and these should be checked separately in conjunction with running the Pharos query. The output indicates benchmark or possible benchmark scores for each human health and environmental endpoint. The output for 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) can be found in Appendix C and a summary of the results can be found below:

- Restricted List
  - VwVwS – Class 1 Low Hazard to Waters

PhysicoChemical Properties of 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime is a liquid at room temperature with a melting point of -20 ºC. Its low vapor pressure indicates that it is unlikely that it will vaporize.

Table 1: Physical and Chemical Properties of 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime (CAS #2224-33-1)

Property	Value	Reference
Molecular formula	C14-H27-N3-O3-Si	ChemIDplus 2014
SMILES Notation	[Si](O\N=C(\CC)C)(O\N=C(\CC)C)(O\N=C(\CC)C)C=C	ChemIDplus 2014
Molecular weight	313.471	ChemIDplus 2014
Physical state	Liquid	ECHA 2014a
Appearance	Straw colored liquid	ECHA 2014a
Melting point	-20 ºC	ECHA 2014a
Vapor pressure	0.025 Pa at 25 ºC (equivalent to 0.0001875 mm Hg[8])	ECHA 2014a
Water solubility	0.00002041 (estimated)	U.S. EPA 2012[9]
Dissociation constant	Not identified	
Density/specific gravity	0.997 g/cm^3 at 20 ºC	ECHA 2014a[9]
Partition coefficient	Log K_{ow} = 10.19	U.S. EPA 2012[9]

[8] 0.025 Pa * 0.0075 = 0.0001875 mm Hg

[9] Note: The EPISuite program (v4.11) developed by the U.S. Environmental Protection Agency and Syracuse Research Corporation has not been validated for silanes that contain silicone in their molecular structure (although some measured data are included in the training data set); therefore, there is uncertainty associated with the calculated values and they should be used with caution.

Hazard Classification Summary Section:

Group I Human Health Effects (Group I Human)

Carcinogenicity (C) Score (H, M, or L): *L*
2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) was assigned a score of Low for carcinogenicity based on modeling results. GreenScreen® criteria classify chemicals as a Low hazard for carcinogenicity when adequate data are available and negative, there are no structural alerts, and they are not GHS classified (CPA 2012a).

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime (CAS# 2224-33-1)
- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- OncoLogic 2013
  - Attempts were made to model the carcinogenicity of 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime using the OncoLogic modeling software program. However, ToxServices was unable to accurately represent its chemical structure. Therefore, modeling using OncoLogic was not completed.
- Toxtree 2013
  - 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime does not have structural alerts for genotoxic or non-genotoxic carcinogenicity. See Appendix D for justification.
- VEGA 2012
  - 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime is predicted to be a non-carcinogen. VEGA notes that the prediction is of low reliability because the compound is out of the model applicability domain. See Appendix E for justification.

2-Butanone, O,O',O''-(methylsilylidyne)trioxime (CAS# 22984-54-9)
- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- No data were identified.

Mutagenicity/Genotoxicity (M) Score (H, M, or L): L
2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) was assigned a score of Low for mutagenicity/genotoxicity based on negative findings in an Ames assay and an *in vivo* micronucleus assay. GreenScreen® criteria classify chemicals as a Low hazard for mutagenicity/genotoxicity when adequate data are available and negative for both chromosomal aberrations and gene mutations, there are no structural alerts, and they are not GHS classified (CPA 2012a).

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime (CAS# 2224-33-1)
- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- UNEP 2009
  - 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime was not mutagenic in an Ames assay conducted according to OECD TG 471 in *S. typhimurium* strains TA98, TA100, TA1535, and TA1537 and *E. coli* WP2 uvrA in the presence and absence of metabolic activation at concentrations of 0, 50, 150, 500, 1,500, and 5,000 µg/plate.

  - In a chromosome aberration assay conducted according to OECD TG 473, Chinese hamster ovary cells were treated with 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime at concentrations between 196 to 3,140 µg/mL without metabolic activation for 4 and 20 hours and 3,140 µg/mL for 4 hours with metabolic activation. Treatment produced a significant increase in structural aberrations in the presence and absence of metabolic activation. Treatment did not induce numerical chromosome aberrations.
  - In an *in vivo* micronucleus test conducted according to OECD TG 474, ICR mice (5/sex) received 450, 900, or 1,800 mg/kg 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime via a single intraperitoneal injection and were sacrificed 24 hours later. An additional group of mice received a single dose of 1,800 mg/kg and were sacrificed 48 hours later. Treated animals were lethargic, had irregular breathing, piloerection, and were prostrating immediately after dose administration. Animals treated with 1,800 mg/kg had palpebral closure after treatment. Animals were lethargic and had piloerection at the end of the treatment period. Treatment did not alter the ratio of polychromatic erythrocytes to total erythrocytes. Treatment caused a reduction in the ratio of polychromatic erythrocytes to total erythrocytes in the bone marrow of male mice treated with 1,800 mg/kg and sacrificed 48 hours later. The authors noted that the lack of bone marrow toxicity in females suggests that the test article may not have reached their bone marrow. Treatment had no effect on the number of micronucleated polychromatic erythrocytes in male or female mice after 24 or 48 hours.

<u>2-Butanone, O,O',O''-(methylsilylidyne)trioxime (CAS# 22984-54-9)</u>

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- UNEP 2009
  - In a chromosome aberration assay conducted according to OECD TG 473, Chinese hamster ovary cells were treated with 2-butanone, O,O',O''-(methylsilylidyne)trioxime at concentrations between 196 and 3,140 µg/mL without metabolic activation for 4 hours and 393 to 3,140 µg/mL with metabolic activation for 20 hours. Treatment did not induce an increase in chromosome aberrations.
- Based on the weight of evidence, a score of Low was assigned. 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime was not mutagenic in an Ames assay and was negative in an *in vivo* micronucleus assay. Mixed results were reported in chromosome aberration assays; 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime induced an increased incidence of structural aberrations while the surrogate did not induce chromosome aberrations in Chinese hamster ovary cells. Although, positive results were reported in an *in vitro* chromosome assay, 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime was not clastogenic *in vivo*; therefore, ToxServices assigned a Low score.

Reproductive Toxicity (R) Score (H, M, or L): L

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) was assigned a score of Low for reproductive toxicity based on negative findings in a reproductive toxicity screening test with the surrogate. GreenScreen® criteria classify chemicals as a Low hazard for reproductive toxicity when there are adequate negative data available, there are no structural alerts, and they are not GHS classified (CPA 2012a).

<u>2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime (CAS# 2224-33-1)</u>

- Authoritative and Screening Lists

  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- No data were identified.

2-Butanone, O,O',O''-(methylsilylidyne)trioxime (CAS# 22984-54-9)

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- UNEP 2009
  - In a combined repeated-dose reproductive/developmental toxicity screening test conducted according to OECD TG 422, Wistar rats received 0, 10, 50, or 250 mg/kg/day 2-butanone, O,O',O''-(methylsilylidyne)trioxime via oral gavage for 28 days (males, 10 animals) or 14 days prior to pairing, throughout pairing and gestation until the F1 mice were 4 days old (females, 10 animals). Treatment had no effect on the fertility index, conception rates, or gestation index. There was no change in the mean duration of gestation. Treatment had no effect on the mean number of implantations or the number of mean post implantation losses. There were no changes in the mean litter size at first check or the sex ratio. No adverse effects were reported. The authors identified a reproductive NOAEL of 250 mg/kg/day (highest dose tested).

Developmental Toxicity incl. Developmental Neurotoxicity (D) Score (H, M, or L): L
2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) was assigned a score of Low for developmental toxicity based on negative findings in a developmental screening test with the surrogate. GreenScreen® criteria classify chemicals as a Low hazard for developmental toxicity when there are adequate negative data available, there are no structural alerts, and they are not GHS classified (CPA 2012a).

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime (CAS# 2224-33-1)

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- No data were identified.

2-Butanone, O,O',O''-(methylsilylidyne)trioxime (CAS# 22984-54-9)

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- UNEP 2009
  - In a previously described combined repeated-dose reproductive/developmental toxicity screening test conducted according to OECD TG 422, Wistar rats received 0, 10, 50, or 250 mg/kg/day 2-butanone, O,O',O''-(methylsilylidyne)trioxime via oral gavage for 28 days (males, 10 animals) or 14 days prior to pairing, throughout pairing and gestation until the F1 mice were 4 days old (females, 10 animals). Treatment had no effect on mean litter size and weight, litter weight gain, pup viability, or sex ratio. Necropsy found no adverse developmental effects. The authors identified a developmental NOAEL of 250 mg/kg/day (highest dose tested).

Endocrine Activity (E) Score (H, M, or L): DG
2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) was assigned a score of Data Gap for endocrine disruption based on a lack of data for this endpoint.

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime (CAS# 2224-33-1)

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- Not listed as a potential endocrine disruptor on the EU Priority List of Suspected Endocrine Disruptors.
- Not listed as a potential endocrine disruptor on the OSPAR List of Chemicals of Possible Concern.
- No data were identified.

2-Butanone, O,O',O''-(methylsilylidyne)trioxime (CAS# 22984-54-9)

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- Not listed as a potential endocrine disruptor on the EU Priority List of Suspected Endocrine Disruptors.
- Not listed as a potential endocrine disruptor on the OSPAR List of Chemicals of Possible Concern.
- No data were identified.

Group II and II* Human Health Effects (Group II and II* Human)

Note: Group II and Group II* endpoints are distinguished in the v 1.2 Benchmark system. For Systemic Toxicity and Neurotoxicity, Group II and II* are considered sub-endpoints and test data for single or repeated exposures may be used. If data exist for single OR repeated exposures, then the endpoint is not considered a data gap. If data are available for both single and repeated exposures, then the more conservative value is used.

Acute Mammalian Toxicity (AT) Group II Score (vH, H, M, or L): M

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) was assigned a score of Moderate for acute toxicity based on an oral LD_{50} in male Fischer 344 rats. GreenScreen® criteria classify chemicals as a Moderate hazard for acute toxicity when oral LD_{50} values are between 300 and 2,000 mg/kg (CPA 2012a).

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime (CAS# 2224-33-1)

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- ECHA 2014a
  - Dermal LD_{50} = > 2,009 mg/kg (male and female Wistar rats)
- UNEP 2009
  - Oral LD_{50} = > 2,000 mg/kg (male Crl: CD (SD) IGS BR VAF/Plus rats)
  - Oral LD_{50} = 1,920 mg/kg (male Fischer 344 rats)
  - Oral LD_{50} = 2,610 mg/kg (female Fischer 344 rats)

2-Butanone, O,O',O''-(methylsilylidyne)trioxime (CAS# 22984-54-9)

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- UNEP 2009
  - Oral LD_{50} = 2,260 mg/kg (male Fischer 344 rats)
  - Oral LD_{50} = 2,650 mg/kg (female Fischer 344 rats)

- Based on the available evidence, a score of Moderate was assigned. 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime had a dermal LD_{50} of greater than 2,009 mg/kg in rats and oral LD_{50} values ranging between 1,920 and 2,610 mg/kg in rats. The surrogate has oral LD_{50} values between 2,260 and 2,650 mg/kg in rats. Based on the oral LD_{50} value of 1,920 mg/kg in male Fischer 344 rats, a score of Moderate was assigned.

Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST)
***Group II Score (single dose)* (vH, H, M, or L): M**
2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) was assigned a score of Moderate for systemic toxicity (single dose) based on findings from an acute toxicity study with the surrogate. GreenScreen® criteria classify chemicals as a Moderate hazard for systemic toxicity (single dose) when the LOAEL is between 300 and 2,000 mg/kg (CPA 2012a).

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime (CAS# 2224-33-1)
- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- No data were identified.

2-Butanone, O,O',O''-(methylsilylidyne)trioxime (CAS# 22984-54-9)
- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- UNEP 2009
  - Fisher 344 rats (5/sex) received 0, 0.3, 1, 2, or 3 mL/kg 2-butanone, O,O',O''-(methylsilylidyne)trioxime via oral gavage and were observed for 14 days. An additional group of rats (5/sex) received 0.3, 1, or 3 mL/kg during the second week of study and were used for hematological investigations on days 1 and 4. Neurobehavioral screening was performed on days 0, 1, 7, and 14. Treatment with 1 mg/kg or greater caused reversible pharmacologic depression of the nervous system. Treatment with 1 mL/kg or greater caused significant oxidative destruction of the red blood cells. All treated animals had splenic changes indicative of erythrolysis. Lymphoid depletion/necrosis was reported in 8/12 spontaneous deaths (1 animal at 1 mL/kg, 3 animals at 2 mL/kg, and 8 animals at 3 mL/kg). Generalized hepatocyte cytoplasmic vacuolation was reported in 5/8 spontaneous deaths at 3 mL/kg. The authors identified LD_{50} values of 2.3 mL/kg (equivalent to 2,260 mg/kg) in males and 2.7 mL/kg (equivalent to 2,650 mg/kg) in females. ToxServices identified a NOAEL of 0.3 mL/kg (equivalent to 295.2 mg/kg[10]) and a LOAEL of 1 mL/kg (equivalent to 984 mg/kg[11]) based on oxidative destruction of the red blood cells.

***Group II* Score (repeated dose)* (H, M, or L):** *H*
2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) was assigned a score of High for systemic toxicity (repeated dose) based on findings in a combined repeated dose/reproductive/developmental screening test for the surrogate. GreenScreen® criteria classify chemicals as a High hazard for systemic toxicity (repeated dose) when the LOAEL equal to or less than 10 mg/kg/day (CPA 2012a).

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime (CAS# 2224-33-1)
- Authoritative and Screening Lists

[10] 0.3 mL/kg * 0.984 g/mL * 1,000 mg/g = 295.2 mg/kg. The density was identified in ECHA (2014c).
[11] 1 mL/kg * 0.984 g/mL * 1,000 mg/g = 984 mg/kg. The density was identified in ECHA (2014c).

  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- No data were identified.

2-Butanone, O,O',O''-(methylsilylidyne)trioxime (CAS# 22984-54-9)

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- UNEP 2009
  - In a previously described combined repeated-dose reproductive/developmental toxicity screening test conducted according to OECD TG 422, Wistar rats received 0, 10, 50, or 250 mg/kg/day 2-butanone, O,O',O''-(methylsilylidyne)trioxime via oral gavage for 28 days (males, 10 animals) or 14 days prior to pairing, throughout pairing and gestation until the F1 mice were 4 days old (approximately 45 days) (females, 10 animals). Treatment caused no deaths and no adverse clinical signs were reported. Hematology measurements could not be completed in rats treated with 250 mg/kg/day due to a dramatic increase in reticulocyte number inhibiting the correct measurement of all other parameters. Animals treated with 50 mg/kg/day had anemia, hemoglobin concentration, decreased hemocrit, increased mean corpuscular volume, increased mean corpuscular hemoglobin, increased reticulocytes, and platelet concentration. Males treated with 250 mg/kg/day had significant increases in urea, sodium, and phosphorus, decreased glucose and potassium, and an increased albumin/globulin ratio. Additionally, their total bilirubin concentration was significantly increased. Females treated with 250 mg/kg/day had significantly decreased glucose, and increased sodium, chloride, and phosphorus. Their albumin/globulin ratio was also increased. All animals treated with 250 mg/kg/day had discolored kidneys and an enlarged spleen. Four males and females treated with 50 mg/kg/day had an enlarged spleen. Males and females treated with 250 mg/kg/day had significant increases in the absolute and relative weights of the heart, liver, and spleen. Treatment with 50 mg/kg/day caused a significant increase in spleen weight in males and females and liver weight in males. Treatment with 50 and 250 mg/kg/day caused hepatocellular hypertrophy, extramedullary hematopoiesis pigmented Kupffer cells, and pigmented cetrilobular hepatocytes in the liver; extramedullary hematopoiesis, hemosiderin deposits and congestion in the spleen; tubular pigment in the kidney; and erythroid hyperplasia in the bone marrow. The authors identified a NOAEL of 10 mg/kg/day and a LOAEL of 50 mg/kg/day base on hematology, blood chemistry, and histopathological findings. *As the guideline values are doubled from 90-day studies to 45-day studies (i.e. 20 and 200 mg/kg/day), there is insufficient data to conclude that adverse effects do not occur at 20 mg/kg/day.*
- Based on the weight of evidence, a score of High was assigned. In the study described above, animals treated with 50 mg/kg/day of the surrogate 2-butanone, O,O',O''-(methylsilylidyne)trioxime had changes in hematology, an enlarged spleen, increased liver and spleen weight, and microscopic changes in the liver, spleen, kidneys and bone marrow. The authors identified a NOAEL of 10 mg/kg/day and a LOAEL of 50 mg/kg/day base on hematology, blood chemistry, and histopathological findings. The difference in treatment duration did not alter the toxicological profile of 2-butanone, O,O',O''-(methylsilylidyne)trioxime, as similar effects were reported in male (28-day treatment) and female rats (~45 day treatment). Therefore, ToxServices doubled the guidance values (i.e., 20 to 200 mg/kg/day) in order to account for the 45-day treatment in female rats. Based on the LOAEL value of 50 mg/kg/day, a score of Moderate should be assigned. However, there is insufficient data to determine if adverse effects occur at doses above the NOAEL of 10 mg/kg/day and at or below the guidance value of 20 mg/kg/day. Therefore, ToxServices

conservatively assigned a High score and reduced the confidence in the endpoint due to insufficient data.

Neurotoxicity (N)
***Group II Score (single dose)* (vH, H, M, or L): M**
2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) was assigned a score of Moderate for neurotoxicity (single dose) based on findings of reversible narcotic effects. GreenScreen® criteria classify chemicals as a Moderate hazard for neurotoxicity (single dose) when classified as GHS Category 3 (CPA 2012a).

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime (CAS# 2224-33-1)

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006, 2014).
- UNEP 2009
  - One male Crl:CD(SD) IGS BR VAF/Plus rat was administered 550 mg/kg 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime via oral gavage and 3 male rats were administered 2,000 mg/kg 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime via oral gavage. Rats were observed for 14 days. Treatment caused no deaths. Treatment produced no adverse effects in animals treated with 550 mg/kg. No adverse effects were reported in two of the three rats treated with 2,000 mg/kg. One male rat treated with 2,000 mg/kg had an absence of or decreased activity, increased lacrimation, partially closed eye lids bilaterally, and irregular respiration rate on the day of dosing. The animal appeared normal by day 3. The authors treated one additional rat with 2,000 mg/kg. The animal had decreased activity on the day of dosing. On the day following dosing the animal had red soiling of the muzzle, bilateral eyes, bilateral forepaws, and clear urogenital staining. The animal appeared normal by day 3. Treatment had no effect on weight gain. Necropsy identified a small focus of the left lateral lobe of the liver of one animal treated with 2,000 mg/kg. The authors identified an LD_{50} of greater than 2,000 mg/kg. ToxServices identified a NOAEL of 550 mg/kg and a LOAEL of 2,000 mg/kg.
  - Fisher 344 rats (5/sex) received 0, 0.3, 1, 2, 3, or 4 mL/kg (equivalent to 295, 990, 1,980, 2,960, and 3,950 mg/kg) via oral gavage and were observed for 14 days. Animals treated with 1 mL/kg and higher had yellow anal/genital staining, decreased respiration, and lacrimation. Chromodacryorrhea was reported in some female animals treated with 2 mL/kg. The authors identified an LD_{50} of 1.94 mL/kg (1,920 mg/kg) in males and 2.64 mL/kg (2,610 mg/kg) in females. ToxServices identified a NOAEL of 0.3 mL/kg (295 mg/kg) and a LOAEL of 1 mL/kg (990 mg/kg).

2-Butanone, O,O',O''-(methylsilylidyne)trioxime (CAS# 22984-54-9)

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006, 2014).
- UNEP 2009
  - In a previously described acute toxicity study, Fisher 344 rats (5/sex) received 0, 0.3, 1, 2, or 3 mL/kg 2-butanone, O,O',O''-(methylsilylidyne)trioxime via oral gavage and were observed for 14 days. An additional group of rats (5/sex) received 0.3, 1, or 3 mL/kg during the second week of study and were used for hematological investigations on days 1 and 4.

Neurobehavioral screening was performed on days 0, 1, 7, and 14. Treatment with 1 mL/kg or greater caused reversible pharmacologic depression of the nervous system. The authors identified LD_{50} values of 2.3 mL/kg (equivalent to 2,260 mg/kg) in males and 2.7 mL/kg (equivalent to 2,650 mg/kg) in females. ToxServices identified a NOAEL of 0.3 mL/kg (equivalent to 299.1 mg/kg[12]) and a LOAEL of 1 mL/kg (equivalent to 997 mg/kg[13]) based on reversible depression of the nervous system.

- Based on the weight of evidence, a score of Moderate was assigned. Acute exposure to 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime or 2-butanone, O,O',O"-(methylsilylidyne)trioxime appears to cause reversible narcotic effects. Clinical signs included decreased activity, increased lacrimation, partially closed eye lids bilaterally, and irregular respiration rate. Animals returned to normal within 3 days. Based on the reversible narcotic effects, 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime was classified as GHS Category 3.

Group II* Score (repeated dose) **(H, M, or L): M**

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) was assigned a score of Moderate for neurotoxicity (repeated dose) based on findings in a combined repeated dose reproductive/developmental toxicity screening test using the surrogate. GreenScreen® criteria classify chemicals as a Moderate hazard for neurotoxicity (repeated dose) when classified as GHS Category 2 (CPA 2012a).

<u>2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime (CAS# 2224-33-1)</u>

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006, 2014).
- No data were identified.

<u>2-Butanone, O,O',O''-(methylsilylidyne)trioxime (CAS# 22984-54-9)</u>

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006, 2014).
- UNEP 2009
  - In a previously described combined repeated-dose/reproductive/developmental toxicity screening test conducted according to OECD TG 422, Wistar rats received 0, 10, 50, or 250 mg/kg/day 2-butanone, O,O',O''-(methylsilylidyne)trioxime via oral gavage for 28 days (males, 10 animals) or 14 days prior to pairing, throughout pairing and gestation until the F1 mice were 4 days old (females, 10 animals). Effects on the nervous system were investigated using the functional observational battery. Male animals treated with 250 mg/kg/day had a decreased number of rearings and decreased mean grip strength of forepaws and hindpaws. Only the decrease in hindpaw strength was significantly significant. Treatment also produced a decreased mean body temperature in males and females treated with 250 mg/kg/day and males treated with 50 mg/kg/day.
- Based on the available data, a score of Moderate was assigned. No neurotoxicity studies were identified for 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime. In a combined repeated dose/reproductive/developmental toxicity screening test animals treated with 250 mg/kg/day 2-

[12] 0.3 mL/kg * 0.997 g/mL * 1,000 mg/g = 299.1 mg/kg
[13] 1 mL/kg * 0.997 g/mL * 1,000 mg/g = 997 mg/kg

butanone, O,O',O''-(methylsilylidyne)trioxime had a decreased number of rearings, and decreased mean grip strength of the forepaws and hindpaws. Additionally, animals treated with 50 and 250 mg/kg/day had decreased body temperature. Therefore, ToxServices classified 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime as GHS Category 2 and assigned a Moderate score.

Skin Sensitization (SnS) Group II* Score (H, M, or L): M
2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) was assigned a score of Moderate for skin sensitization based on positive findings in a guinea pig maximization study. GreenScreen® criteria classify chemicals as a Moderate hazard for skin sensitization when classified as GHS Category 1B (CPA 2012a).

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime (CAS# 2224-33-1)
- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- No data were identified.

2-Butanone, O,O',O''-(methylsilylidyne)trioxime (CAS# 22984-54-9)
- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- ECHA 2014a
  - 2-Butanone, O,O',O''-(methylsilylidyne)trioxime was sensitizing in a GLP-compliant guinea pig maximization study conducted according to OECD Guideline 406. Female Hartley guinea pigs (3 controls/15 test) were induced with 2 intradermal injections of 5% of the test article followed by an epicutaneous injection of 25% of the test article. Animals were challenged with a single dermal exposure to 50% of the test article. Fourteen of 15 animals treated with 2-butanone, O,O',O''-(methylsilylidyne)trioxime had positive skin reactions at 24 and 48 hours. In the negative control group, 1 of 3 animals had a positive skin reaction at 24 hours and 0 of 3 animals had a positive skin reaction at 48 hours.
- Based on the weight of evidence, a score of Moderate was assigned. 2-butanone, O,O',O''-(methylsilylidyne)trioxime caused skin sensitization in 93% of tested animals (14/15) which warrants classification as GHS Category 1B.

Respiratory Sensitization (SnR) Group II* Score (H, M, or L): DG
2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) was assigned a score of Data Gap for respiratory sensitization based on a lack of data for this endpoint.

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime (CAS# 2224-33-1)
- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- No data were identified.

2-Butanone, O,O',O''-(methylsilylidyne)trioxime (CAS# 22984-54-9)
- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- No data were identified.

Skin Irritation/Corrosivity (IrS) Group II Score (vH, H, M, or L): *M*
2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) was assigned a score of Moderate for skin irritation/corrosivity based on findings in skin irritation studies. GreenScreen® criteria classify chemicals as a Moderate hazard for skin irritation/corrosivity when classified as GHS Category 2 (CPA 2012a).

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime (CAS# 2224-33-1)

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- UNEP 2009
  - New Zealand white rabbits were dermally exposed to undiluted 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime for 24 hours under semi-occlusive conditions (intact-skin). Treatment produced necrosis in 2/6 animals; however, the necrosis was superficial and reversible. No dermal irritation was reported by day 8. The authors reported a primary dermal irritation index of 2.7. Individual scores were not reported. The authors reported 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime was moderately irritating.

2-Butanone, O,O',O''-(methylsilylidyne)trioxime (CAS# 22984-54-9)

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- UNEP 2009
  - Rabbits (strain not reported) were dermally exposed to undiluted 2-butanone, O,O',O''-(methylsilylidyne)trioxime for 24 hours under occlusive conditions (intact skin). Four animals had erythema 1 hour after patch removal. Erythema was resolved within 72 hours. Four animals had signs of edema 1 hour after patch removal which was resolved within 48 hours. The authors reported a primary dermal irritation index of 0.5. Individual scores were not reported. The authors reported that 2-butanone, O,O',O''-(methylsilylidyne)trioxime is slightly irritating.
- Based on the weight of evidence, a score of Moderate was assigned. Dermal exposure to 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime under semi-occlusive conditions for 24 hours caused reversible necrosis and no dermal irritation was reported after 8 days. The study description did not indicate if treatment caused dermal irritation prior to day 8. The authors of the SIDS Dossier stated 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime was moderately irritating. Dermal exposure to 2-butanone, O,O',O''-(methylsilylidyne)trioxime caused erythema and edema in animals that was reversible within 73 and 48 hours, respectively. The authors of the SIDS Dossier stated 2-butanone, O,O',O''-(methylsilylidyne)trioxime is slightly irritating. Individual erythema or edema scores were not reported for either study. Therefore, ToxServices classified 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) as GHS Category 2 (mild irritant) based on the presence of erythema and edema following treatment with 2-butanone, O,O',O"-(methylsilylidyne)trioxime and descriptions made in the SIDS Dossier of moderately and slightly irritating. Confidence was reduced due to a lack of detail in the study descriptions.

Eye Irritation/Corrosivity (IrE) Group II Score (vH, H, M, or L): H
2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) was assigned a score of High for eye irritation/corrosivity based on findings of eye irritation studies. GreenScreen® criteria classify

chemicals as a High hazard for eye irritation/corrosivity when classified as GHS Category 2A (CPA 2012a).

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime (CAS# 2224-33-1)

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- UNEP 2009
  - Undiluted 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime was instilled into the conjunctival sac of New Zealand white rabbits (9 animals). The eyes of 3 animals were washed approximately 20 seconds after instillation. The eyes of the remaining 6 animals were not washed. Animals with unwashed eyes had corneal opacity at 1 hour and 1 day following treatment; it was resolved in 4 animals by day 7, but persisted in 2 animals for 21 days. Iritis was reported in 2 animals within 1 hour and 1 day after treatment; it resolved within 2 days. Conjunctival redness, chemosis, and discharge were reported in all animals 1 hour after treatment. Chemosis was resolved in all animals within 2 days; redness was resolved in all animals but 1 within 14 days and the remaining animal within 21 days; discharge was resolved in all animals except 1 by day 4 and in the remaining animal by day 10. The authors stated the results for animals with washed eyes were similar except that irritation resolved in all eyes by 14 days. They stated that 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime is severely irritating to the eyes.
- ECHA 2014a
  - 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime was irritating to the eyes of New Zealand White rabbits (6 animals) in a GLP-compliant acute eye irritation study conducted according to OECD Guideline 405. One-hundred microliters of the test substance was instilled into one eye of rabbits and they were observed for 72 hours. Five of the 6 treated animals had an average conjunctivae score after 72 hours of 2.0 and an average cornea score after 72 hours of 2.0. All treated animals had an average iris score of 1. As animals were only observed for 72 hours it is not known if these effects were reversible within 21 days.

2-Butanone, O,O',O''-(methylsilylidyne)trioxime (CAS# 22984-54-9)

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- UNEP 2009
  - Undiluted 2-butanone, O,O',O''-(methylsilylidyne)trioxime was instilled into one eye of rabbits (strain not reported) (9 animals). The eyes of 3 animals were washed 20 seconds after treatment and the remaining 6 animals had unwashed eyes. Treatment caused corneal opacity, circumcorneal injection of the iris, conjunctival redness, chemosis, and discharge in 5 of 6 animals with unwashed eyes within 24 hours. These effects were reversible within 7 days. Two of the 3 animals with rinsed eyes did not have ocular irritation. The authors stated 2-butanone, O,O',O''-(methylsilylidyne)trioxime was moderately irritating to rabbit eyes.
  - Undiluted or 2-butanone, O,O',O''-(methylsilylidyne)trioxime diluted in peanut oil (30%, 10%, 3%) was instilled into one eye of New Zealand white rabbits (6 males). Undiluted 2-butanone, O,O',O''-(methylsilylidyne)trioxime was slightly irritating and animals showed lachrymal secretions and congestion and edema of the conjunctival membrane. These effects were reversed within 24 hours and congestion cleared within 4 to 5 days. Dullness of the cornea was reported in 3 animals, however it quickly cleared. Diluted (30%) 2-

butanone, O,O',O''-(methylsilylidyne)trioxime caused some lacrylmal secretions and slight congestion for 6 hours. The authors stated that 2-butanone, O,O',O''-(methylsilylidyne)trioxime is slightly irritating to irritating to rabbit eyes.

- Based on the weight of evidence, a score of High was assigned. Ocular exposure to 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime produced corneal opacity, iritis, conjunctival redness, chemosis, and discharge in rabbits. The ECHA study indicated that five of the six treated animals had an average (24-72 hrs) conjunctivae score of 2 and a cornea score of 2, while all animals had and iris score of 1. These irritation scores warrant classification as GHS Category 2A. Authors of the SIDS Dossier stated 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime is severely irritating to rabbit eyes. Ocular exposure to 2-butanone, O,O',O''-(methylsilylidyne)trioxime caused corneal opacity, circumcorneal injection of the iris, conjunctival redness, chemosis, and discharge in rabbits. No individual scores were reported. Authors of the SIDS Dossier stated 2-butanone, O,O',O''-(methylsilylidyne)trioxime was slightly irritating to moderately irritating to rabbit eyes. Based on the available evidence 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime was classified as GHS Category 2A.

Ecotoxicity (Ecotox)

Acute Aquatic Toxicity (AA) Score (vH, H, M, or L): M
2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) was assigned a score of Moderate for acute aquatic toxicity based on findings of an acute toxicity study in algae using the surrogate. GreenScreen® criteria classify chemicals as a Moderate hazard for acute aquatic toxicity when acute toxicity values are between 10 and 100 mg/L (CPA 2012a).

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime (CAS# 2224-33-1)

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- No data were identified.

2-Butanone, O,O',O''-(methylsilylidyne)trioxime (CAS# 22984-54-9)

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- UNEP 2009
  - 96h LC_{50} = > 120 mg/L (nominal) (*oncorhynchus mykiss,* fish)
  - 48h EC_{50} = > 120 mg/L (nominal) (*Daphnia magna,* daphnia)
  - 72h EyC_{50} (biomass) = 50 mg/L (nominal) (*Pseudokirchneriella subcapitata,* algae)
  - 72h EC_{50} (cell density) = 50 mg/L (nominal) (*Pseudokirchneriella subcapitata,* algae)

Chronic Aquatic Toxicity (CA) Score (vH, H, M, or L): DG
2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) was assigned a score of Data Gap for chronic aquatic toxicity based on a lack of data for this endpoint.

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime (CAS# 2224-33-1)

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- No data were identified.

2-Butanone, O,O',O''-(methylsilylidyne)trioxime (CAS# 22984-54-9)

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- No data were identified.

Environmental Fate (Fate)

Persistence (P) Score (vH, H, M, L, or vL): L

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) was assigned a score of Low for persistence based on expert judgment. GreenScreen® criteria classify chemicals as a Low hazard for persistence when the half-life in soil, sediment, or water is less than 16 days (CPA 2012a).

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime (CAS# 2224-33-1)

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- UNEP 2009
  - 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime is expected to hydrolyze rapidly (less than 1 minute at pH 7 and 2ºC).
- U.S. EPA 2012
  - Fugacity modeling predicts 81.2% will partition to soil with a half-life of 75 days, 17.6% will partition to water with a half-life of 37.5 days, and 0.805% will partition to sediment with a half-life of 337.5 days (Appendix F).[14]

2-Butanone, O,O',O''-(methylsilylidyne)trioxime (CAS# 22984-54-9)

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- UNEP 2009
  - 2-Butanone, O,O',O''-(methylsilylidyne)trioxime hydrolyzes rapidly with a half-life of less than 1 minute at pH 7 and 2 ºC.
- Based on the weight of evidence, a score of Low was assigned for Persistence. 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) is expected to hydrolyze rapidly with a half-life of less than 1 minute. BIOWIN modeling predicts that it will partition primarily to soil with a half-life of 75 days. However, EPISuite has not been validated for silanes; therefore, the predicted half-life was not considered in the scoring of this endpoint. As moisture is present in soil, 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) is also expected to hydrolyze rapidly in soil. Therefore, ToxServices assigned a score of Low based on the expected rapid hydrolysis of 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) in soil. Potential hazards from relevant and feasible transformation products are discussed previously in this GreenScreen® assessment.

[14] Note: The EPISuite program (v4.11) developed by the U.S. Environmental Protection Agency and Syracuse Research Corporation has not been validated for silanes that contain silicone in their molecular structure (although some measured data are included in the training data set); therefore, there is uncertainty associated with the calculated values and they should be used with caution.

Bioaccumulation (B) Score (vH, H, M, L, or vL): vL
2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) was assigned a score of Very Low for bioaccumulation based on expert judgment . GreenScreen® criteria classify chemicals as a Very Low hazard for bioaccumulation when the BCF is less than 100 (CPA 2012a).

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime (CAS# 2224-33-1)
- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- UNEP 2009
  - Due to the rapid hydrolysis of 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime, the BCF is predicted to be low. A measured BCF of the hydrolysis product methylethylketoxime (CAS# 96-29-7) in fish ranges between 0.5 to less than 2.5.

2-Butanone, O,O',O''-(methylsilylidyne)trioxime (CAS# 22984-54-9)
- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists

Physical Hazards (Physical)

Reactivity (Rx) Score (vH, H, M, or L): L
2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) was assigned a score of Low for reactivity based on findings that it is not explosive or oxidizing. GreenScreen® criteria classify chemicals as a Low hazard for reactivity when they are not explosive or oxidizing (CPA 2012a).

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime (CAS# 2224-33-1)
- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- ECHA 2014a
  - 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime was not explosive in a GLP-compliant explosive properties study (EU Method A.14).
- ECHA 2014b
  - 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime is not oxidizing (GLP, EU Method A.21).

2-Butanone, O,O',O''-(methylsilylidyne)trioxime (CAS# 22984-54-9)
- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists

Flammability (F) Score (vH, H, M, or L): *M*
2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) was assigned a score of Moderate for flammability based on the flash point. GreenScreen® criteria classify chemicals as a Moderate hazard for flammability when classified as GHS Category 4 (CPA 2012a).

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime (CAS# 2224-33-1)
- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists

  - *Screening:* not on any screening lists
- ECHA 2014a
  - 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime has a flash point > 99 ºC at 1013 hPa (closed cup) (ASTM D 3278).
- ECHA 2014b
  - 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime has a flash point of 91 ºC at 101.4 kPa (GLP, EU Method A.9).

<u>2-Butanone, O,O',O''-(methylsilylidyne)trioxime (CAS# 22984-54-9)</u>

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists
  - *Screening:* not on any screening lists
- Based on the weight of evidence, a score of Moderate was assigned. Two flashpoints were identified for 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime. ToxServices conservatively classified 2-butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime as GHS Category 4 based on the flashpoint of 91 ºC. Confidence in this endpoint was reduced due to inconsistency in the data.

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APPENDIX A: Hazard Benchmark Acronyms
(in alphabetical order)

(AA) Acute Aquatic Toxicity

(AT) Acute Mammalian Toxicity

(B) Bioaccumulation

(C) Carcinogenicity

(CA) Chronic Aquatic Toxicity

(D) Developmental Toxicity

(E) Endocrine Activity

(F) Flammability

(IrE) Eye Irritation/Corrosivity

(IrS) Skin Irritation/Corrosivity

(M) Mutagenicity and Genotoxicity

(N) Neurotoxicity

(P) Persistence

(R) Reproductive Toxicity

(Rx) Reactivity

(SnS) Sensitization- Skin

(SnR) Sensitization- Respiratory

(ST) Systemic/Organ Toxicity

APPENDIX B: Results of Automated GreenScreen® Score Calculation for 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) (CAS #2224-33-1)

TOXSERVICES
TOXICOLOGY RISK ASSESSMENT CONSULTING

GreenScreen® Score Inspector

Table 1: Hazard Table

	Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
	Carcinogenicity	Mutagenicity/Genotoxicity	Reproductive Toxicity	Developmental Toxicity	Endocrine Activity	Acute Toxicity	Systemic Toxicity		Neurotoxicity		Skin Sensitization*	Respiratory Sensitization*	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation	Reactivity	Flammability
							S	R *	S	R *	*	*								
Table 2: Chemical Details																				
Inorganic Chemical?	**Chemical Name**	**CAS#**	**C**	**M**	**R**	**D**	**E**	**AT**	**STs**	**STr**	**Ns**	**Nr**	**SNS***	**SNR***	**IrS**	**IrE**	**AA**	**CA**	**P**	**B**	**Rx**	**F**
No	2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime)	2224-33-1	*L*	**L**	**L**	**L**	DG	**M**	**M**	*H*	**M**	**M**	**M**	DG	*M*	**H**	**M**	DG	**L**	**vL**	**L**	*M*

Table 3: Hazard Summary Table

Benchmark	a	b	c	d	e	f	g
1	No	No	No	No	No		
2	No	No	No	No	No	Yes	No
3	STOP						
4	STOP						

Table 4

Chemical Name	Preliminary GreenScreen® Benchmark Score
2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime)	2

Note: Chemical has not undergone a data gap assessment. Not a Final GreenScreen™ Score

Table 6

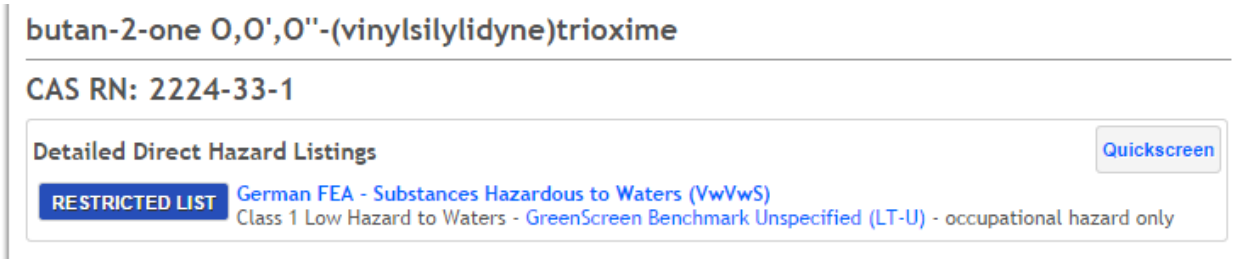
Chemical Name	Final GreenScreen® Benchmark Score
2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime)	2

After Data gap Assessment
Note: No Data gap Assessment Done if Preliminary GS Benchmark Score is 1.

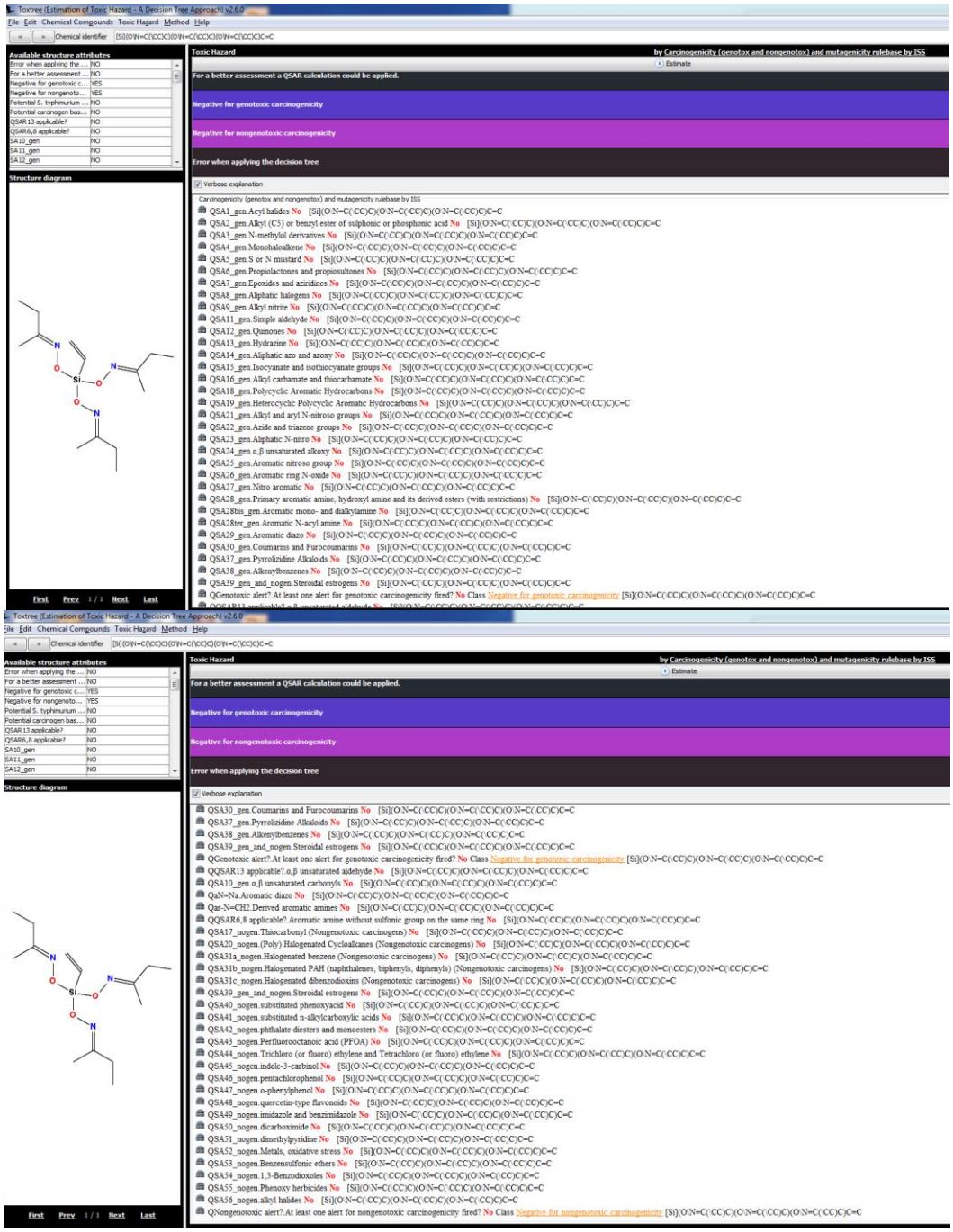
Table 5: Data Gap Assessment Table

Datagap Criteria	a	b	c	d	e	f	g	h	i	j	bm4	End Result
1												
2	Yes	Yes	Yes	Yes	Yes							2
3												
4												

APPENDIX C: Pharos Output for 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) (CAS #2224-33-1)



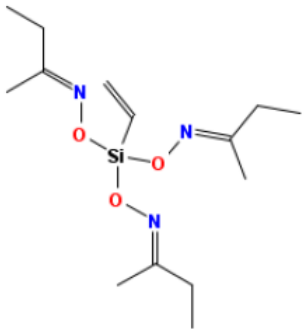
APPENDIX D: ToxTree Modeling Results for 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) (CAS #2224-33-1)



APPENDIX E: VEGA Modeling Results for 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) (CAS #2224-33-1)

1. Prediction Summary

Prediction for compound 1 (Molecule 1)

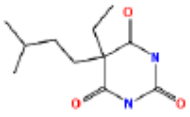


Prediction: Reliability:

Model assessment: Prediction is NON-Carcinogen, but the result may be not reliable. Careful check of the information given in the following section should be done, paying particular attention to the following issues:
- only moderately similar compounds with known experimental value in the training set have been found
- some similar molecules found in the training set have experimental values that disagree with the predicted value
- a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments

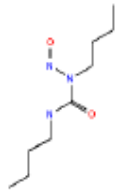
Compound: 1
Compound SMILES: N(O[Si](ON=C(C)CC)(ON=C(C)CC)C=C)=C(C)CC
Experimental value: -
Prediction: NON-Carcinogen
Carcinogen: 0.37
NON-Carcinogen: 0.63
Structural Alerts: -
Reliability: Compound is out of model Applicability Domain
Remarks for the prediction:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



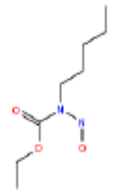
CAS: 57-43-2
Dataset id: 51 (training set)
SMILES: O=C1NC(=O)C(C(=O)N1)(CC)CCC(C)C
Similarity: 0.687

Experimental value: NON-Carcinogen
Predicted value: NON-Carcinogen



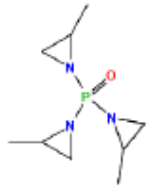
CAS: 56654-52-5
Dataset id: 216 (training set)
SMILES: O=NN(C(=O)NCCCC)CCCC
Similarity: 0.683

Experimental value: Carcinogen
Predicted value: Carcinogen



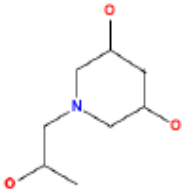
CAS: 64005-62-5
Dataset id: 571 (test set)
SMILES: O=NN(C(=O)OCC)CCCCC
Similarity: 0.678

Experimental value: Carcinogen
Predicted value: Carcinogen



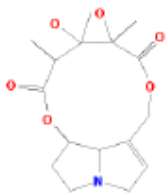
CAS: 57-39-6
Dataset id: 431 (training set)
SMILES: O=P(N1CC1C)(N2CC2C)N3CC3C
Similarity: 0.672

Experimental value: Carcinogen
Predicted value: NON-Carcinogen



CAS: 122-20-3
Dataset id: 785 (training set)
SMILES: OC(C)CN(CC(O)C)CC(O)C
Similarity: 0.669

Experimental value: NON-Carcinogen
Predicted value: NON-Carcinogen



CAS: 315-22-0
Dataset id: 488 (test set)
SMILES: O=C1OC3CCN2CC=C(COC(=O)C(O)(C)C(O)(C)C1C)C23
Similarity: 0.669

Experimental value: Carcinogen
Predicted value: Carcinogen

3.2 Applicability Domain:
Measured Applicability Domain Scores

✖	**Global AD Index** AD Index = 0.279 Explanation: predicted substance is outside the Applicability Domain of the model.
⚠	**Similar molecules with known experimental value** Similarity index = 0.685 Explanation: only moderately similar compounds with known experimental value in the training set have been found.
⚠	**Concordance for similar molecules** Concordance index = 0.502 Explanation: some similar molecules found in the training set have experimental values that disagree with the predicted value.
✔	**Accuracy of prediction for similar molecules** Accuracy index = 1 Explanation: accuracy of prediction for similar molecules found in the training set is good.
✖	**Atom Centered Fragments similarity check** ACF matching index = 0.4 Explanation: a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments.
✔	**Model assignment reliability** Pos/Non-Pos difference = 0.267 Explanation: model class assignment is well defined.
✔	**Neural map neurons concordance** NN concordance = 1 Explanation: predicted value agrees with experimental values of training set compounds laying in the same neuron.
✔	**Model descriptors range check** Descriptors range check = true Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set.

Symbols explanation:

✔ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✖ The feature has a bad assessment, model is not reliable regarding this aspect.

APPENDIX F: EPISuite Modeling Results for 2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) (CAS #2224-33-1)

CAS Number: (null)
SMILES : [Si](ON=C(CC)C)(ON=C(CC)C)(ON=C(CC)C)C=C
CHEM :
MOL FOR: C14 H27 N3 O3 Si1
MOL WT : 313.48
---------- EPI SUMMARY (v4.11) ----------

Physical Property Inputs:
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
Vapor Pressure (mm Hg) : ------
Water Solubility (mg/L): ------
Henry LC (atm-m3/mole) : ------

Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.68 estimate) = 10.19

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
Boiling Pt (deg C): 340.58 (Adapted Stein & Brown method)
Melting Pt (deg C): 12.26 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 0.000221 (Modified Grain method)
VP (Pa, 25 deg C) : 0.0294 (Modified Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.42):
Water Solubility at 25 deg C (mg/L): 2.041e-005
log Kow used: 10.19 (estimated)
no-melting pt equation used

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 0.0068926 mg/L

ECOSAR Class Program (ECOSAR v1.11):
Class(es) found:
Neutral Organics

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method : 4.96E-003 atm-m3/mole (5.02E+002 Pa-m3/mole)
Group Method: Incomplete
For Henry LC Comparison Purposes:
User-Entered Henry LC: not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 4.466E+000 atm-m3/mole (4.525E+005 Pa-m3/mole)
VP: 0.000221 mm Hg (source: MPBPVP)
WS: 2.04E-005 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:
Log Kow used: 10.19 (KowWin est)
Log Kaw used: -0.693 (HenryWin est)
Log Koa (KOAWIN v1.10 estimate): 10.883
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model) : 0.5983
Biowin2 (Non-Linear Model) : 0.1911
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 2.5064 (weeks-months)
Biowin4 (Primary Survey Model) : 3.3955 (days-weeks)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model) : -0.0512
Biowin6 (MITI Non-Linear Model): 0.0065
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.2161
Ready Biodegradability Prediction: NO

Hydrocarbon Biodegradation (BioHCwin v1.01):
Structure incompatible with current estimation method!

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 0.0295 Pa (0.000221 mm Hg)
Log Koa (Koawin est): 10.883
Kp (particle/gas partition coef. (m3/ug)):
Mackay model : 0.000102
Octanol/air (Koa) model: 0.0187
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model : 0.00366
Mackay model : 0.00808
Octanol/air (Koa) model: 0.6

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 30.7501 E-12 cm3/molecule-sec
Half-Life = 0.348 Days (12-hr day; 1.5E6 OH/cm3)
Half-Life = 4.174 Hrs
Ozone Reaction:
OVERALL Ozone Rate Constant = 0.175000 E-17 cm3/molecule-sec
Half-Life = 6.549 Days (at 7E11 mol/cm3)
Fraction sorbed to airborne particulates (phi):
0.00587 (Junge-Pankow, Mackay avg)
0.6 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):
Koc : 5.933E+005 L/kg (MCI method)
Log Koc: 5.773 (MCI method)

Koc : 6.974E+008 L/kg (Kow method)
Log Koc: 8.844 (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:
Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.01):
Log BCF from regression-based method = 2.562 (BCF = 364.8 L/kg wet-wt)
Log Biotransformation Half-life (HL) = 2.6299 days (HL = 426.5 days)
Log BCF Arnot-Gobas method (upper trophic) = 1.452 (BCF = 28.31)
Log BAF Arnot-Gobas method (upper trophic) = 5.051 (BAF = 1.125e+005)
log Kow used: 10.19 (estimated)

Volatilization from Water:
Henry LC: 0.00496 atm-m3/mole (estimated by Bond SAR Method)
Half-Life from Model River: 2.016 hours
Half-Life from Model Lake : 170.4 hours (7.102 days)

Removal In Wastewater Treatment:
Total removal: 94.04 percent
Total biodegradation: 0.78 percent
Total sludge adsorption: 93.26 percent
Total to Air: 0.00 percent
(using 10000 hr Bio P,A,S)

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.323	7.93	1000
Water	17.6	900	1000
Soil	81.2	1.8e+003	1000
Sediment	0.805	8.1e+003	0

Persistence Time: 1.06e+003 hr

Sources to Check for GreenScreen® Hazard Assessment

Note: For a GreenScreen® Hazard Assessment, data queries should be initially limited to the following references. If data gaps exist after these references have been checked, additional references may be utilized.

U.S. EPA High Production Volume Information System (HPVIS):
http://www.epa.gov/hpvis/index.html

UNEP OECD Screening Information Datasets (SIDS):
http://www.chem.unep.ch/irptc/sids/OECDSIDS/sidspub.html

OECD Existing Chemicals Database: http://webnet.oecd.org/hpv/ui/SponsoredChemicals.aspx

European Chemical Substances Information System IUCLID Chemical Data Sheets:
http://esis.jrc.ec.europa.eu/index.php?PGM=dat

National Toxicology Program: http://ntp.niehs.nih.gov/

International Agency for the Research on Cancer:
http://monographs.iarc.fr/ENG/Classification/index.php

Human and Environmental Risk Assessment (HERA) on ingredients of household cleaning products:
http://www.heraproject.com/RiskAssessment.cfm

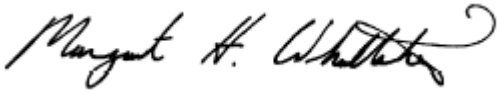
European Chemicals Agency (ECHA) REACH Dossiers: http://echa.europa.eu/

Licensed GreenScreen® Profilers

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) GreenScreen® Evaluation Prepared By:

Sara M. Ciotti, Ph.D.
Toxicologist
ToxServices LLC

2-Butanone, 2,2',2''-(O,O',O''-(ethenylsilylidyne)trioxime) GreenScreen® Evaluation QC'd By:



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