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Your Ref:
Our Ref: 5036759/23/MAS

27 October 2010

Ms Claire Sproats
South Cambridgeshire District Council
South Cambs Hall
Cambourne Business Park
Cambourne
Cambridge
CB3 6EA

Dear Claire,

Former Bayer CropScience, Hauxton: Risk Assessment of Contaminants Not Previously Identified; Grid Cell H11, H12, H13 and J15 (CNPI letter no. 5)

Further characterisation sampling and analysis have identified two contaminants not previously identified (CNPIs) requiring further assessment and derivation of Remedial Targets. These CNPIs were notified to South Cambridgeshire District Council by Harrow Estates (28.09.2010 and 05.10.2010).

The grid squares in which the CNPI has been identified, and the treatment beds in which the materials have been placed, are summarised in Table 1. The CNPIs will be added to the contaminants of concern verification list for both the respective grid cells in which the CNPIs were identified and the corresponding treatment beds. The grid squares are shown on the enclosed Site Survey Reference Grid plan.

Table 1 – CNPIs Requiring Further Assessment and Derivation of Remedial Targets

Contaminant		Grid squares	Treatment beds
Oxathiane 4,4-dioxide	(CAS 107-61-9)	H13	TB111, TB112, TB114
Indane	(CAS 496-11-7)	H12	TB113-114, TB116

The compounds presented in Table 2 are CNPIs that have been risk assessed previously and for which Remedial Targets have already been derived. The CNPIs will be added to the list of verification sampling priority contaminants for the relevant grid cell and corresponding treatment beds.

Table 2 – CNPIs Risk Assessed in previous CNPI reports

Contaminant	Grid squares	Treatment beds
Trichloro methyl benzene (trichloro toluene)	H10, H13, I9, I10, I11, I14 J10, J11, K13	TB6, TB46-47, TB59-60, TB63, TB77, TB83-84, TB87-88, TB93-100, TB102, TB104, TB106, TB108-109, TB111-114
Dichloromethylphenol	H7, H10, H13, I9, I10, I11, I15, J10, J11, J12, K10, K12, K13, L11, L12	TB6, TB17-18, TB23, TB30-31, TB46-47, TB50-51, TB53, TB59-60, TB63, TB67, TB69, TB70a, TB70b, TB71, TB73, TB77-80, TB83-88, TB91-102, TB104-106, TB108-109, TB111-114
1-(2-Chloroethoxy)-2-(o-Tolyloxy)-ethane (CAS 21120-80-9)	H13, I9, J10, K13	TB6, TB46-47, TB59-60, TB63, TB84, TB87, TB94, TB96, TB99-100, TB111-112, TB114

Ethyltoluene (ethyl methyl benzene)	H12, J14	TB1, TB105, TB113-114, TB116
Bis methylpropyl phenol	H12, J16	TB1, TB4, TB107, TB113-114, TB116

Four further compounds were identified, however these were encountered and assessed during the site investigation and were deemed not to be priority contaminants.

Toxicological assessments and human health and controlled waters risk assessments have been carried out for the new CNPI and, where sufficient toxicological, physical and chemical data is available, preliminary Remedial Targets have been derived. The preliminary Remedial Targets will be provided to Vertase, who currently intend to use these for the CNPI.

Where there is insufficient toxicological, physical and chemical data available for assessment and modelling, suitable surrogate compounds for which Remedial Targets have already been derived for the Hauxton site have been identified and selected based on chemical structures and toxicity data, see Table 3. Where surrogates have been adopted and identified for a particular CNPI, the actual CNPI be measured and assessed against the Remedial Target for the surrogate.

Table 3 – Surrogates Used

Contaminant	Surrogates	
	Human Health	Controlled Waters
Oxathiane 4,4-dioxide	Benzene	-
Indane	Aromatic TPH C8-10	-

The CNPI Remedial Targets and required laboratory limits of detection (LODs) are summarised in Table 4. As for the previously identified contaminants of concern, four Remedial Targets have been derived for the CNPI: i) treated materials which will be placed within 20m of Riddy Brook (Inner Zone), ii) treated materials which will be placed at least 20m from Riddy Brook (Outer Zone), iii) treated materials which will be placed at least 1 m below final site levels, after levels have been raised to account for flood risk, (controlled waters risk driven) and iv) treated materials which will be placed within 1 m of final site levels (human health risk driven). The CNPIs and derived/surrogate Remedial Targets will be added to the list of Contaminants of Concern for the relevant grid square and treatment bed validation suites.

Table 4 – Preliminary Remedial Targets

Contaminant	*Remedial Targets* (µg/kg)				LOD (µg/kg)
	Greater than 1m depth		Less than1m depth		
	Outer Zone	Inner Zone	Outer Zone	Inner Zone	
Oxathiane 4,4-dioxide	10	10	10	10	10
Indane	100,000	Do not place in inner zone	1590	Do not place in inner zone	100

The data collected, methods and models used in the derivation of Remedial Targets and identification of surrogates are detailed in Annex 1: Derivation of Generic Assessment Criteria for the protection of Human Health, Annex 2: Surrogate Selection Summary, Annex 3:

Derivation of Generic Assessment Criteria for the Protection of *C*ontrolled Waters and Annex 4: Controlled Waters Modelling Outputs.

The treatability of this compound has been reviewed by Vertase FLI and the remediation of the CNPI will be dealt with by the existing treatment train identified in the Remediation Method Statement (Version 6) and detailed in the Environmental Permit Deployment Form for the site.

Yours sincerely
For and on behalf of Atkins Limited

Mark Smith
Project Manager

Cc Eileen Young – Environment Agency
Nigel Blazeby - South Cambridgeshire District Council

Enc.

A1

Legend

Site Boundary

Rev.	Description	Revised By	Date
B	Text Rotated	JWH	21-04-10
A	Text added in Grid Squares	JWH	01-04-10
	FIRST ISSUE		19-02-10

Vertase F.L.I.

■ Bristol Head Office: Tel: 01275 397600 Fax: 01275 397601

□ Sheffield Office: Tel: 01246 813289 Fax: 01246 812963

□ Hertford Office: Tel: 01992 535757 Fax: 01992 535858

□ Manchester Office: Tel: 01614 372708 Fax: 01614 376300

email: info@vertaseffli.co.uk
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Site Address:

Bayer Site
Hauxton
Cambridge

Rev: B

Title: Site Survey Reference Grid

Client: Harrow Estates

Drawn: JWH	Checked: JWH	Approved: CL
Dwg: D907_56	Contract: 907 BRI	Scale: 1:1250

Annex 1: Derivation of Generic Assessment Criteria for the Protection of Human Health

Introduction

Laboratory analysis from soil characterisation at the site has identified two compounds not previously identified (CNPI). These compounds did not have available generic assessment criteria (GAC). The CNPIs are:

- Oxathiane-4,4-dioxide (CAS No. 107-61-9)
- Indane (CAS No. 496-11-7)

Due to a lack of toxicological data, the following steps were undertaken in order to assign a surrogate for the assessment of this compound, as outlined below.

Methodology

The derivation of any GAC involves a number of steps including a toxicological assessment and the collation of physical and chemical data for each contaminant. In the derivation of such criteria the Environment Agency has released three guidance documents, namely:

- Science Report (SR)2 – Human Health toxicological assessment of contaminants in soil;
- SR3 – Updated technical background to the CLEA model; and
- SR7 – Compilation of Data for Priority Organic Pollutants for Derivation of Soil Guideline Values.

Following the methodology outlined in these documents, Atkins has carried out a toxicological search for the identified CNPIs. However, the surrogate allocation process did not result in the need for a detailed review of all the physical and chemical input parameters required for the derivation of soil assessment criteria for these compounds. The process of surrogate allocation is discussed in further detail below.

Toxicology

Oxathiane-4,4-dioxide

In order to evaluate Oxathiane-4,4-dioxide appropriately, a search for toxicological data was undertaken. The search was conducted as described in the Environment Agency's *Human Health toxicological assessment of contaminants in soil – Science Report SC050021/SR2*, particularly an evaluation of the available data from all 33 sources listed, as advised. There was insufficient information available in order to derive a suitable HCV for use in a further assessment. Therefore, a suitable surrogate was identified using the information available based on similarities in structure, toxicity and physical and chemical data.

The comparison of structures included evaluation of all compounds previously assessed at the site during earlier phases of the project, as well as chemicals evaluated at other sites and the available soil screening value (SSV) suite of chemicals. The most suitable were then selected on the basis of basic structure, as well as similarity of additional chemical groups and substituent groups such as nitro, halogen, hydroxyl and alkyl groups. Those deemed most suitable were then compared initially on the basis of relative toxicity. Once a shortlist was drawn

up on the basis of similarity in structure, the relative toxicity of each chemical was also considered.

Following on from the comparison of structure and relative toxicity, specific chemical and physical parameters were evaluated to make sure that estimated exposure to the surrogate would not be significantly lower than that of the chemical of concern (CoC).

Physical and Chemical Data

Following the preliminary search for toxicological data, it was decided that a surrogate compound would be assigned. Therefore, the Henry's Law Constant (HLC) and log octanol-water coefficient (log Kow) were chosen as the most relevant physical and chemical parameters for surrogate selection. These parameters would aid in an evaluation of potential exposure to the receptor, in the absence of detailed exposure modelling. There was a paucity of data within the the seven data sources that the Environment Agency presented in SR7., Indicative values for these two parameters were therefore obtained from the Estimation Programs Interface (EPI) Suite from the United States (US) Environmental Protection Agency (EPA).

The HLC was used as an indication of a chemical's tendency to partition between soil air and soil water, and therefore its tendency to be present in ambient and indoor air. A chemical of concern (CoC) with a higher HLC than its chosen surrogate will, under the same atmospheric conditions, usually be present in higher concentrations in soil vapour. Therefore, the comparison of HLC was done in order to ensure that the CoC would not be more likely to partition to soil air than its chosen surrogate.

In a similar manner, the log Kow was used to determine the potential for a compound to partition to lipid phase, and therefore to be present within home grown produce.

Further information on the surrogate selection is presented in Annex 2.

Indane

In order to evaluate indane appropriately, a search for toxicological data was undertaken. The search was conducted on similar principles to those described in the Environment Agency's *Human Health toxicological assessment of contaminants in soil – Science Report SC050021/SR2*, particularly an evaluation of the available data from the majority of the 33 sources listed, as advised. The checklist showing the toxicological sources used for this research has been included in Annex 2.

There was insufficient information available in order to derive suitable Health Criteria Values (HCVs) for use in a further assessment of this compound. However, indane has been observed to be a component of the total petroleum hydrocarbon (TPH) compounds, with an equivalent carbon number of 10, as listed within the Total Petroleum Hydrocarbon Criteria Working Group (TPHCWG) Series Composition of Petroleum Mixtures - Volume 2 (API, 1998). It would therefore be reasonable to assume that it will be present within the aromatic TPH C8-10 fraction. It is also assumed that this compound contributes to the toxicological effect of this group of compounds and was considered by the TPHCWG during the derivation of the toxicological benchmarks used by Atkins to develop the HCVs for this fraction. Therefore, the toxicology data and physical and chemical data used to derive a GAC for the aromatic TPH C8-10 fraction will be suitably conservative for the assessment of indane. Therefore, Atkins considers that the aromatic TPH C8-10 fraction will be a suitably conservative surrogate for indane. In order to assess this compound, the measured concentration of indane should be assessed in conjunction with other components of this fraction. In effect, it can be assumed to be contained within the reported concentration of aromatic TPH C8-10 measured at the site. However, where the aromatic TPH C8-10 fraction is not measured within soils, the reported

concentration of indane should be added to reported concentrations of all other compounds that are considered likely to be contained in this fraction from a specific soil sample, and compared to the relevant GAC.

Results and conclusions

The results of surrogate selection are presented in Table 1 below. The presented GACs are based on the GACs derived for the allocated surrogates.

Table 2 - Summary of Surrogate Selection

Compound	Selected Surrogate	GAC mg/kg
oxathiane-4,4-dioxide	benzene	4.93E-02
Indane	Aromatic TPH C8-10	1.59*

* This GAC refers to the aromatic TPH C8-10 group, and the measured concentration of this compound can be assumed to be contained within the reported concentration of aromatic TPH C8-10 measured at the site. Where the aromatic TPH C8-10 fraction is not measured within soils, the reported concentration of this compound should be added to that of all other compounds that are considered likely to be contained in the fraction, and the sum total compared to the GAC.

References

Estimation Programs Interface (EPI), 2009. EPI SuiteTM by the U.S. Environmental Protection Agency. Available from 26/08/2010: http://www.epa.gov/oppt/exposure/pubs/episuitedl.htm

American Petroleum Institute (API), 1998. Total Petroleum Hydrocarbon Criteria Working Group (TPHCWG). Volume 2 - Series Composition of Petroleum Mixtures.

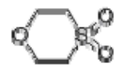
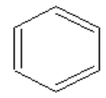
Environment Agency, 2008. Compilation of Data for Priority Organic Pollutants for Derivation of Soil Guideline Values Science Report Final SC050021/ SR7.

Environment Agency, 2009a. Human Health toxicological assessment of contaminants in soil. Science Report Final SC050021/SR2.

Environment Agency, 2009b. Updated technical background to the CLEA model Science Report Final SC050021/SR3.

Annex 2: Surrogate Selection Summary

ANNEX 2 - SURROGATE SELECTION SUMMARY

Chemical name	CAS Number	Structure	Available tox data	Henry's law Constant (HLC)	Log Kow	Suggested Surrogate(s)	Surrogate Inhalation HCV (mg/m³)	Surrogate selected	Justification
Oxathiane-4,4-dioxide	107-61-9		LD50 - 200mg/kg	4.33E-003 Pa-m³/mole 1.75E-006 unitless 4.28E-008 atm-m³/mole	1.4924	chlorobenzene, 4-chloro-2-methylphenol, benzene, cyclohexanone	0.483, 0.112, 0.0049, 0.1358	 **Benzene (HLC dimensionless 0.116; Log Kow 2.13. Ref: EA, 2008; Lethal dose of 50-500 mg/kg in humans. Ref: HSDB, 2010)),**	There is a paucity of readily available toxicity data for this chemical. In the absence of suitable toxicity data, the most conservative of the structurally similar compounds, benzene, has been selected as a potential surrogate. The limited acute toxicity data also indicate that it is likely to be of similar toxicity to benzene over an acute exposure period. Benzene is therefore selected as a surrogate for this compound.

Environment Agency (EA), 2008 Compilation of Data for Priority Organic Pollutants for Derivation of Soil Guideline Values. Science Report:SC050021/SR7
Hazardous Substances data bank, 2010. Available from: http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~lTtc7p:1

Rechecked IPCS - website errors

SOURCE DATA CHECK LIST

Chemical name: **Indane**

Common name: Indane; Indan

CAS RN: 496-11-7

Source	Checked? (Y/N)	Type of Data found
UK Sources		
Food Standards Agency	Y	None
Health Protection Agency	Y	None
Health and Safety Executive	Y	None
Health and Safety Laboratory	Y	—
UK Drinking Water Inspectorate	Y	—
Pesticide Safety Directorate	Y	None
COC	Y	None
COM	Y	~
COT	Y	~
COMEAP	Y	~
Expert panel an Air Quality Standards	Y	~
EU Sources		
European Chemicals Bureau	Y	None
European Food Safety Authority	Y	✓
ECETOC	Y	✓
International		
IPCS INCHEM:	✓YES	Nothing under search of indane on main chemical sheet – except for some petroleum hydrocarbon documents which popped up, none of which had TDIs in there. One had ecotox issues
IARC	✓	None
PIM	✓	✓
EHC	✓	✓
HSG	✓	✓
PDS	✓	✓
JECFA	✓	✓
JMPR	✓	✓
OECD SIDS	Y	None

CICADS	✓ Y	None
WHO:		
Guidelines for DW Quality	✓ Y	None
Air Quality Guidelines for Europe	✓ Y	None
	Foreign National	
RIVM MPR	Y	None
Health Canada Tox Ref Values	Y	None
US EPA:	—	
AEGL	—	
Health Advisories	—	
IRIS		None
Tox Ref Database	—	
ATSDR	—	
	Other	
TOXNET (including TERA)	Y	Looked at ITER - nothing ; checked entire TOXNET; chem I.D. only
Pubmed	—	—

Type of Data Found: This section should contain the following codes for easy classification of data found. Acronym should be separated with ';' or '/'

CID: Chemical Identification
TKn: Toxicokinetics (data on absorption, distribution, metabolism and excretion round the organism)
AT: Acute Toxicity
SaT: Subacute Toxicity (short term repeat dose studies)
ScT: Subchronic Toxicity (longer-term studies)
CT: Chronic Toxicity (long-term toxicity data)
RT: Reproductive Toxicity
DT: Developmental Toxicity (specific to developmental effects in offspring)
GT: Genotixicity
C: Carcinogenicity
O: Other

Originated By: _Hannah_____ **Date:** __5th October 2010_____

Checked By: ___TA_____ **Date:** 12/10/2010

Annex 3: Derivation of Generic Assessment Criteria the Protection of Controlled Waters

This annex provides an initial assessment of the substances detected at the Former Agrochemical works, Main Site at Hauxton, near Cambridge with respect to risk to controlled waters receptors.

The CNPIs are listed in the following table:

Chemical Name	CAS Number	Chemical Formula
Indane	496-11-7	C_9H_{10}
Oxathiane-4,4-dioxide	107-61-9	$C_4H_8O_3S$

This annex provides a summary of the physical and chemical properties of this substance, and an assessment of its potential risk to controlled waters using a qualitative or quantitative risk assessment method as appropriate. Either a surrogate substance is selected from amongst the existing priority contaminants for controlled waters (qualitative) if appropriate to the CNPI; or a specific remedial target for the substance has been calculated (quantitative) using the methodology developed in 2007 (Ref 1).

Indane

Synonyms: *Indan, hydroindene*

This substance is a polyaromatic hydrocarbon (PAH) consisting of a benzene ring sharing two carbons with a 5 carbon ring. The 5 carbon ring does not include a double bond within it. The molecule is one of the smallest PAH molecule and looks superficially similar to naphthalene, however naphthalene comprises two joined benzene rings. Two other relatively small PAHs which include a similar 5 carbon ring are acenaphthene and fluorene. These two substances contain two benzene rings along with a 5 carbon ring in differing arrangements.

The physical and chemical properties of Indane pertaining to contaminant transport in groundwater, from literature sources, are as follows:

Properties	Units	Values	Reference
Henry's Law	Pa m^3/mol	214	Montgomery, J.H., 2007. Groundwater Chemicals Desk Reference. Fourth Edition. Boca Raton, Florida: CRC Press.
Log K_{OW}	-	3.18 – 3.57	Range of literature values from Mackay D., Shiu W.Y., Lee S.C. and Ma K. Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals, Second Edition Aug 2006 (CD-ROM).
Log K_{OC}	-	3.13 – 3.51	Converted from K_{OW} using equation 70 from Ref 2.
K_{OC}	-	1337 - 3233	Converted from log K_{OC}

Properties	Units	Values	Reference
Half Life (Anaerobic)	days	258* - 365	258 days is the longest literature quoted half life of the PAHs naphthalene, acenaphthene or fluorene in groundwater from Mackay D., Shiu W.Y., Lee S.C. and Ma K. Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals, Second Edition Aug 2006 (CD-ROM).

$T_{1/2}$ naphthalene

There is considered to be sufficient published data on the properties of indane, to generate a conservative remedial target. The risk assessment to calculate the remedial target assumes a worst case (longest) half life for similar PAHs (naphthalene, fluorene or acenaphthene) in groundwater as a minimum value. Naphthalene has a longer biodegradation half life quoted from the literature (258 days) than either fluorene or acenaphthene, therefore it assumed that the 5 carbon ring may be a less table structure than a benzene ring. As a margin of safety a range of half lives has been considered between 258 and 365 days for indane.

The compliance concentration at the receptor used was 0.1µg/l (the UK Drinking Water Standard for PAHs). The methodology used to calculate the target was the same as used in the 2007 risk assessment (Ref 1).

Oxathiane-4,4-dioxide

Synonyms: 1,4lambda6-oxathiane-4,4-dione, 1,4-oxathiane 4,4-dioxide, 1,4-thioxane 1,1-dioxide, 4,4-dioxo-1,4-oxathiane, P-thioxanesulfone, Thioxanesulfone, Usafdo-38, 1,4-thioxane-1,1-dioxide

This substance comprises a 6 sided cyclic structure consisting of four carbons, an oxygen and a sulphur atom. The ring is not a benzene ring as it does not consist of 6 carbons with a dissociated bond between. The oxygen is in the position of the first carbon in the ring and the sulphur is in the 4th position. There are then two oxygen atoms doubled bonded to the sulphur, hence “4,4-dioxide” in the name of this substance.

No information on the contaminant transport properties of this substance have been found from the literature source surveyed. It has been possible to simulate the potential contaminants transport properties of this substance using EPIWIN and BioWin software which have been used to produce the predicted values in the table below.

Properties	Units	Values	Reference
Henry’s Law	Unitless	1.75×10^{-6}	EPIWIN Prediction
Log K_{OW}	-	-1.4924	EPIWIN Prediction
Log K_{OC}	-	-1.467	Converted from Log K_{OW} using equation 70 from Ref 2.
K_{OC}	-	0.034	Converted from Log K_{OC}
Half Life (Anaerobic)	days	14 - 31	BioWIN predictions suggest substance should not readily biodegrade. Values selected on an un-conservative basis to demonstrate risk.

Oxathiane-4,4-dioxide is very different in its constituents and structure (sulphur and oxygen within a hydrocarbon ring) when compared with any of the other substances considered in the risk screening carried out in 2007 (Ref. 1).

The use of surrogate substance to provide remedial targets is therefore not a reasonable possibility. It is considered that the only remedial target which could be set for oxathiane-4,4-dioxide would be a target based on the simulated parameters determined through use of EPIWIN and BioWIN. The results of the BioWIN modelling are open to interpretation, BioWIN4 suggests that the substance may degrade on a time scale of weeks to days, however BioWIN7 suggests the substance is unlikely to readily biodegrade under anaerobic conditions. A relatively un-conservative range of biodegradation rates have been selected to demonstrate the potential risks posed by this substance using estimated contaminant transport values. The results of the remedial target calculations are considered to demonstrate that the only justifiable targets for this substance are the detection limits that could be reliably achieved by a commercial laboratory.

The potential sensitivity of this substance to controlled waters cannot be quantified based on the current information available therefore a limit of 0.1µg/l at the compliance point has been assessed, which is considered to be a stringent limit of detection.

Summary

In summary the following recommendations are made as a result of screening the potential risks associated to controlled waters with regard to the substances detected by TIC GCMS screening at the Hauxton Main Site.

Sufficient data on the contaminant transport properties of Indane were available for a species specific remedial target to be derived for indane. Estimated properties were used to assess the remedial target for oxathiane-4,4-dioxide due to a lack of published information on its likely properties. No surrogates are considered similar oxathiane-4,4-dioxide. The results of the remedial target assessment for oxathiane-4,4-dioxide suggest that the only justifiable target for this substance are considered to be the detection limits that could be reliably achieved by a commercial laboratory.

The table below lists the CNPIs calculated remedial targets.

Substances	Priority Contaminant Surrogates	Target Concentration (µg/kg)	
		Inner Zone	Outer Zone
Indane	-	>10^	100,000#
Oxathiane-4,4-dioxide	-	>10*	>10**

^ Calculated target concentration of 3.83 µg/kg. A limit of 10 µg/kg has been applied as a limit of detection that can be reliably achieved by a commercial laboratory.

Calculated Target Concentration 2.1×10^6µg/kg

* Calculated target concentration of 0.0175 µg/kg. A limit of 10 µg/kg has been applied as a limit of detection that can be reliably achieved by a commercial laboratory.

** Calculated target concentration of 7.21 µg/kg. A limit of 10 µg/kg has been applied as a limit of detection that can be reliably achieved by a commercial laboratory.

References

1 Atkins Ltd; Groundwater Modelling Report; Remediation of Former Bayer Site, Hauxton; February 2007

2 US EPA Document: EPA/540/R-95/128 (July 1996). Soil Screening Guidance: Technical Background Document.

Annex 4: Controlled Waters Modelling Outputs

107-61-9

Log Kow(version 1.67 estimate): -1.49

SMILES : O=S(=O)(CCOC1)C1
CHEM : 1,4-Oxathiane, 4,4-dioxide
MOL FOR: C4 H8 O3 S1
MOL WT : 136.17

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	4	-CH2- [aliphatic carbon]	0.4911	1.9644
Frag	1	-O- [oxygen, aliphatic attach]	-1.2566	-1.2566
Frag	1	-SO2- [sulfone, aliphatic attach]	-2.4292	-2.4292
Const		Equation Constant		0.2290

Log Kow = -1.4924

Bond Est : 4.28E-008 atm-m3/mole (4.33E-003 Pa-m3/mole)
Group Est: Incomplete

SMILES : O=S(=O)(CCOC1)C1
CHEM : 1,4-Oxathiane, 4,4-dioxide
MOL FOR: C4 H8 O3 S1
MOL WT : 136.17

HENRYWIN v3.20 Results

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	8 Hydrogen to Carbon (aliphatic) Bonds		-0.9574
FRAGMENT	2 C-C		0.2326
FRAGMENT	2 C-O		2.1709
FRAGMENT	2 C-S		2.2112
FRAGMENT	2 O=S (sulfone-type)	ESTIMATE	2.1000
RESULT	BOND ESTIMATION METHOD for LWAPC VALUE	TOTAL	5.757

HENRYs LAW CONSTANT at 25 deg C = 4.28E-008 atm-m3/mole
= 1.75E-006 unitless
= 4.33E-003 Pa-m3/mole

	GROUP CONTRIBUTION DESCRIPTION	COMMENT	VALUE

```
--------+---------------------------------------------+------------+--------
        |         2  CH2 (C)(O)                       |          | -0.26
        |         2  CH2 (C)(S)                       |          | -0.04
        |         1  O (C)(C)                         |          |  2.93
        |           MISSING Value for:  S (=O)(C)(C)(=O)
--------+---------------------------------------------+------------+--------
 RESULT |  GROUP ESTIMATION METHOD for LOG GAMMA VALUE  |
INCOMPLETE |  2.63
--------+---------------------------------------------+------------+--------
```

107-61-9

Results of BioWIN

SMILES : O=S(=O)(CCOC1)C1
CHEM : 1,4-Oxathiane, 4,4-dioxide
MOL FOR: C4 H8 O3 S1
MOL WT : 136.17
---------- BIOWIN v4.10 Results ----------

Biowin1 (Linear Model Prediction) : Does Not Biodegrade Fast
Biowin2 (Non-Linear Model Prediction): Does Not Biodegrade Fast
Biowin3 (Ultimate Biodegradation Timeframe): Weeks
Biowin4 (Primary Biodegradation Timeframe): Days-Weeks
Biowin5 (MITI Linear Model Prediction) : Not Readily Degradable
Biowin6 (MITI Non-Linear Model Prediction): Not Readily Degradable
Biowin7 (Anaerobic Model Prediction): Does Not Biodegrade Fast
Ready Biodegradability Prediction: NO

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic ether [C-O-C]	-0.3474	-0.3474
MolWt	*	Molecular Weight Parameter		-0.0648
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		0.3354

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic ether [C-O-C]	-3.4294	-3.4294
MolWt	*	Molecular Weight Parameter		-1.9336
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.0867

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	Biowin3 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic ether [C-O-C]	-0.0087	-0.0087
MolWt	*	Molecular Weight Parameter		-0.3009
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		2.8896

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic ether [C-O-C]	-0.0097	-0.0097
MolWt	*	Molecular Weight Parameter		-0.1965
Const	*	Equation Constant		3.8477
RESULT		Biowin4 (Survey Model - Primary Biodeg)		3.6415

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks
(Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic ether [C-O-C]	0.0015	0.0015
Frag	4	-CH2- [cyclic]	0.0197	0.0789
MolWt	*	Molecular Weight Parameter		-0.4051
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.3874

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic ether [C-O-C]	-0.1071	-0.1071
Frag	4	-CH2- [cyclic]	0.2365	0.9461
MolWt	*	Molecular Weight Parameter		-3.9310

```
============+==========================================+=====
====+=========
  RESULT   |Biowin6 (MITI Non-Linear Biodeg Probability)|        | 0.3621
============+==========================================+=====
====+=========
```

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

```
------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |      Biowin7 FRAGMENT DESCRIPTION       | COEFF  | VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Aliphatic ether  [C-O-C]               | -0.2573 | -0.2573
 Frag |  4  |  -CH2-  [cyclic]                        | -0.1200 | -0.4801
 Const|  *  |  Equation Constant                      |         | 0.8361
============+==========================================+=====
====+=========
  RESULT   |   Biowin7 (Anaerobic Linear Biodeg Prob)   |        | 0.0988
============+==========================================+=====
====+=========
```

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

Results of BioHCwin

SMILES : O=S(=O)(CCOC1)C1
CHEM : 1,4-Oxathiane, 4,4-dioxide
MOL FOR: C4 H8 O3 S1
MOL WT : 136.17
---------- BioHCwin v1.01 Results ----------

NO Estimate Possible ... Structure NOT a Hydrocarbon
(Contains atoms other than C, H or S (-S-))