Ethyl Xanthate

Ethyl Xanthate is one of these chemicals where no or little data is available regarding their environmental impact. This chemical substance is not classified in the Annex I of Directive 67/548/EEC. The chemical fate and pathways of Ethyl Xanthate to the environment has not been assessed before along with its PBT status. An assessment of the PBT status of Ethyl Xanthate using the algorithm described in the toolbox is explained below step by step

Step1: Substance identification

Identifiers on Ethyl Xanthate have been obtained from the most recent reliable sources (www.chemfinder.com and chemID plus) which are listed in step1. These identifiers are shown in Table1 below. The smiles notation for Ethyl Xanthate was obtained from chemIDplus and Chemspider sources.

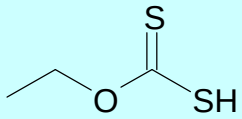
Identifier of Ethyl Xanthate	
EINECS or ELINCS number	205-780-8
CAS name and CAS number	151-01-9
Name(s) in the IUPAC nomenclature or other international chemical name(s)	Carbonic acid, dithio-, O-ethyl ester Carbonodithioic acid, O-ethyl ester O-Ethyl hydrogen dithiocarbonate
Other names (usual name, trade name, abbreviation)	Ethoxydithioformic acid Ethyl xanthate Ethyl xanthogenate Ethylxanthic acid Ethylxanthogenic acid
Information related to molecular and structural formula of Ethyl Xanthate	
Molecular Formula	C3-H6-O-S2
Structural formula	
Smiles Notation	O(C(S)=S)CC

Table1: Ethyl Xanthate identification parameters.

Step 2: Data needed for the assessment

These are divided into the followings:

- Physical-chemical properties (water solubility, Partition coefficient n-octanol/water, Soil Adsorption Coefficient (Koc/Kd), and Henry's Law Constant)
- Degradation, (biodegradation, half lives)
- Accumulation (BCF)
- Environmental Partitioning (MacKay)
- Ecotoxicity data of the substance (LC_{50}, NOEC)

Step3: Collecting the available information and identifying the data gap

1- Information on the physical-chemical properties for Ethyl Xanthate

The following table provides a summary of the

1. Chemical and physical properties required for the assessment as explained in the algorithm.
2. The available chemical and physical properties of Ethyl Xanthate along with the source for these data. As explained in the algorithm, in this step you have to make sure that the data studies were conducted according to EU-approved methods (e.g. those specified in Annexes V and VIII of Directive 67/548/EEC, or REACH Annex X methods) and in compliance with the principles of GLP. This only applies for degradation, accumulation and ecotoxicity studies not for the physical-chemical one.
3. The data gap which is highlighted as red in the table.

Required Property	Value	Source
Water solubility	slightly sol in water	HSDB
Partition coefficient n-octanol/water		
Soil Adsorption Coefficient (Koc/Kd)		

Henry's Law Constant		

Table2: Physical chemical data available for Ethyl Xanthate.

2- Accumulation data of Ethyl Xanthate

No accumulation data are available.

3- Degradation data of Ethyl Xanthate

The following table provides a summary of the

1. Degradation properties required for the assessment as explained in the algorithm.
2. The available degradation data of Ethyl Xanthate along with the source for these data. As explained in the algorithm, the data should be reliable.
3. The data gap which is highlighted as red in the table.

Required Property	**Value**	**Source**
Biodegradation		
Half lives-$t_{1/2}$		
1-Hydrolysis as a function of Ph		
2-Photolysis (Atmospheric OH Rate Constant)		

Table3: Degradation data available for Ethyl Xanthate.

4- Environmental Partitioning (MacKay)

No data found.

5- Aquatic toxicity information of Ethyl Xanthate

No data found

Step 4: Filling the data gap by using QSAR

In this step the above endpoints (both the available and not) will be predicted using QSARs tools and software listed in step 4 of this algorithm (EPIWIN, Danish(Q)SAR data base and PBT profiler). The reason for doing this is to compare the QSAR results with the experimental one to identify the accuracy of the QSAR.

1- Results obtained by using EPIWIN

Table 4 provides the predicted values for the above endpoints using EPIWIN software along with the name of the programme used. The output obtained by EPIWIN for each end point is given. Also included are explanations which could be obtained by clicking on the link below to view.

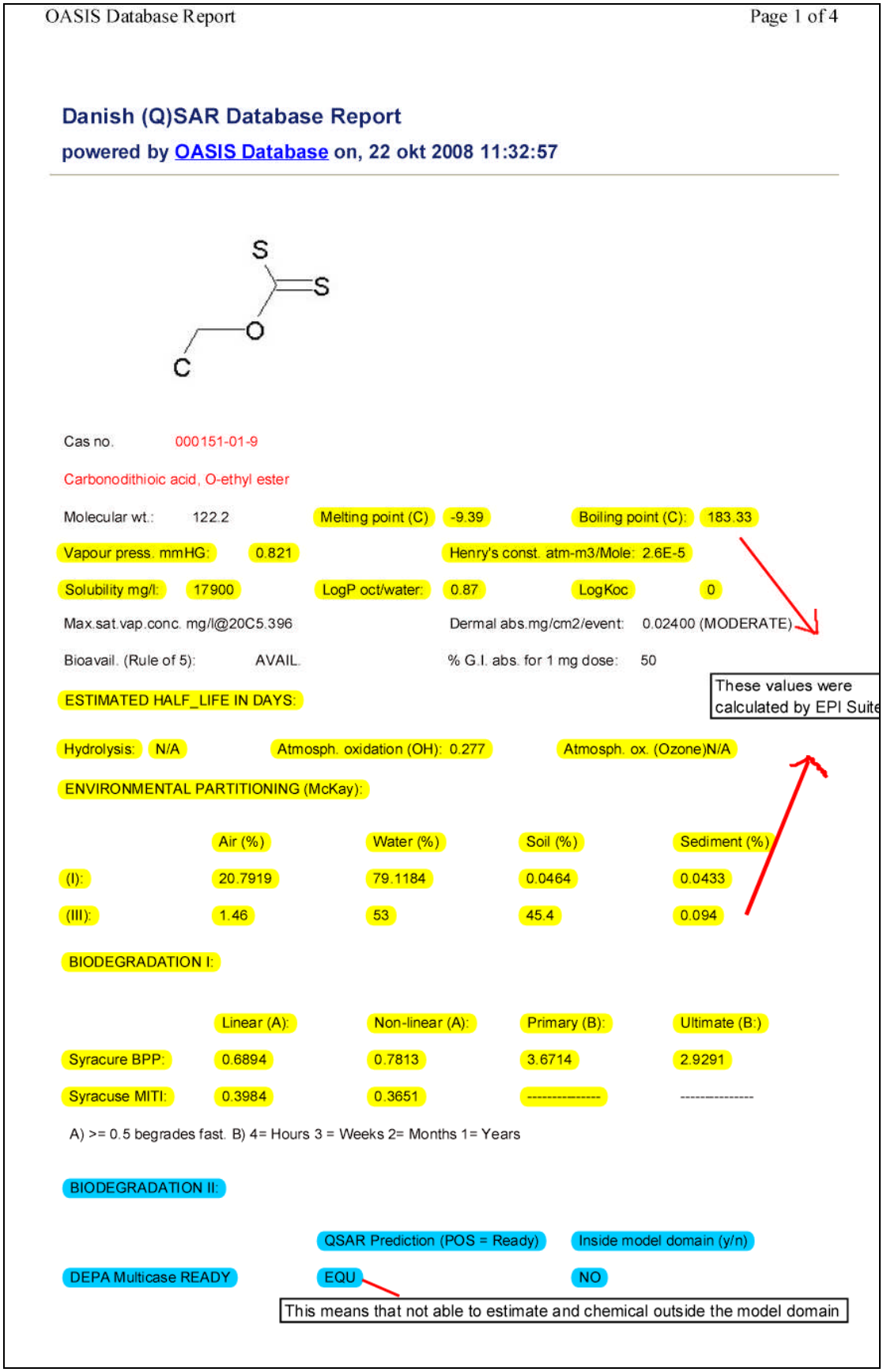
Required Property	**EPI QSAR Programme**	**Predicted Value**
Water solubility	WSKOW	1.79e+004 mg/l at 25 C
Partition coefficient n-octanol/water	KOWWIN	Log K_{ow} = 0.87
Bioconcentration Factor (BCF)	BCFWIN	LogBCF = 0.5 (BCF = 3.16)
Soil Adsorption Coefficient (Koc/Kd)	(PCKOCWIN)	K_{oc} = 1
Henry's Law Constant	HENRYWIN	2.60 * 10^{-5}atm-m^3/mole
Half lives-$t_{1/2}$		
1-Hydrolysis as a function of pH	HYDROWIN	Can not be estimated
2-Photolysis (Atmospheric OH Rate Constant)	AOPWIN	Atmospheric Oxidation Rate Constant = 37.2E-12 cm^3/molecule-sec Half-Life = 3.44 hrs
(Atmosph. Oxidation, Ozone)	AOPWIN	Can not be estimated
Biodegradability		
BIOWIN1	BIOWIN	0.69 (Biodegrades fast)
BIOWIN2	BIOWIN	0.78 (biodegrades fast)
BIOWIN3 (Ultimate biodegradation)	BIOWIN	2.93 (weeks)
BIOWIN4 (Primary Biodegradation)	BIOWIN	3.67 (Days)
BIOWIN5	BIOWIN	0.39 (not readily degradable)
BIOWIN6	BIOWIN	0.37 (not readily degradable)

BIOWIN7	BIOWIN	0.78 (Does not Biodegrade fast)
Ready Biodegradability Prediction:	BIOWIN	No
Environmental Partitioning		
(MacKay)	EPI V3.2	Level III Fugacity Model: Mass Amount (percent) / Half-Life (hr) Air 1.23 / 6.64 Water 45.7 / 360 Soil 53 / 720 Sediment 0.089 / 3.24e+003
Fish Acute toxicity to fish (96hrs LC50) mol/l Long term toxicity (28days NOEC) mol/l	ECOSAR	LC_{50} (96hrs) = 1045 mg/l ChV(30days)= 112 mg/l, where CHV is chronic toxicity value
Daphnia Acute toxicity to Daphnia (48hrs EC_{50}) mol/l Long term toxicity (21days NOEC) mol/l	ECOSAR	LC_{50} (48hrs) = 1036 mg/l
Algae Acute toxicity to Algae (72hrs EC_{50}) mol/l	ECOSAR	EC_{50} (96-hr) = 606 mg/l

Table4: EPIWIN predictions of the required endpoints

2- Results obtained from Danish(Q)SAR database

The Danish (Q)SAR report for Ethyl Xanthate is shown below (Figures 1 and 2) with some comments. This output contains predictions for physical-chemical, environmental and human health endpoints, however, as we are only interested in selected physical-chemical endpoints along with the environmental endpoints these are highlighted in yellow or blue in the report. The yellow highlighter identifies the values that have been predicted in the Danish (Q)SAR using the EPIWIN suite and therefore we can check whether the results obtained directly with the EPIWIN suite agree (Table 5). The blue highlighter indicates to the values predicted using other QSAR models such as multicase which is used to predict the biodegradability.



Danish (Q)SAR Database Report

powered by OASIS Database on, 22 okt 2008 11:32:57

Cas no. 000151-01-9

Carbonodithioic acid, O-ethyl ester

Molecular wt.: 122.2 Melting point (C) -9.39 Boiling point (C): 183.33

Vapour press. mmHG: 0.821 Henry's const. atm-m3/Mole: 2.6E-5

Solubility mg/l: 17900 LogP oct/water: 0.87 LogKoc 0

Max.sat.vap.conc. mg/l@20C5.396 Dermal abs.mg/cm2/event: 0.02400 (MODERATE)

Bioavail. (Rule of 5): AVAIL. % G.I. abs. for 1 mg dose: 50

These values were calculated by EPI Suite

ESTIMATED HALF_LIFE IN DAYS:

Hydrolysis: N/A Atmosph. oxidation (OH): 0.277 Atmosph. ox. (Ozone)N/A

ENVIRONMENTAL PARTITIONING (McKay):

	Air (%)	Water (%)	Soil (%)	Sediment (%)
(I):	20.7919	79.1184	0.0464	0.0433
(III):	1.46	53	45.4	0.094

BIODEGRADATION I:

	Linear (A):	Non-linear (A):	Primary (B):	Ultimate (B:)
Syracure BPP:	0.6894	0.7813	3.6714	2.9291
Syracuse MITI:	0.3984	0.3651	----------	----------

A) >= 0.5 begrades fast. B) 4= Hours 3 = Weeks 2= Months 1= Years

BIODEGRADATION II:

	QSAR Prediction (POS = Ready)	Inside model domain (y/n)
DEPA Multicase READY	EQU	NO

This means that not able to estimate and chemical outside the model domain

Figure1: Danish (Q)SAR report for Ethyl Xanthate.

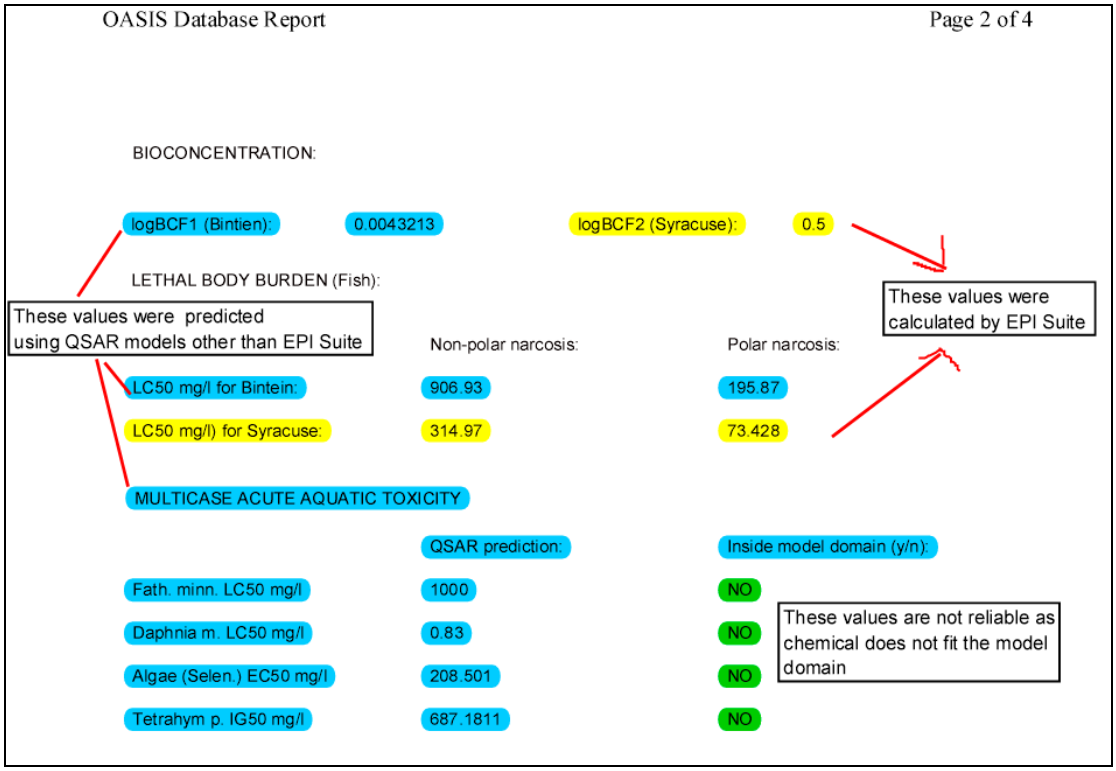


Figure2: Danish (Q)SAR report for Ethyl Xanthate.

Before proceeding to step 5, it is useful to compare the predicted values obtained from EPIWIN and the Danish(Q)SAR database with the experimental data (see Table 5). As well as checking the accuracy of the methodology, the reproducibility of EPIWIN predictions can be tested as explained previously.

Unfortunately no experimental data is available to compare with. From Table 5 we could see that the predictions from the EPIWIN suite are consistent with the one obtained from the Danish(Q)SAR as expected (Log K_{ow}, Log K_{oc} and Henry's Law Constant, see Table 5). In addition, the predicted parameters from using QSARs other than EPIWIN which are listed in Danish(Q)SAR report are also approximately close to EPIWIN estimates in terms of classification. An example for this can be seen in the BCF estimate. However, the prediction of the biodegradability using mutlicase could not be determined as chemical does not fit the model domain for this programme.

Required Property	**Predicted Value using Danish database**	**Predicted Value using EPIWIN**
Water solubility	17900 mg/l	1.79e+004 mg/l at 25 C
Partition coefficient n-octanol/water	log K_{ow} = 0.87	Log K_{ow} = 0.87
Bioconcentration Factor (BCF)	LogBCF2 (Syracuse) = 0.5 Log BCF(Bintien) = 0.00432 (BCF = 1.00999)	LogBCF = 0.5 (BCF = 3.16)
Soil Adsorption Coefficient (Koc/Kd)	log Koc = 0, K_{oc} = 1	K_{oc} = 1
Henry's Law Constant	2.6 *10^{-5}atm-m^3/mole	2.60 * 10^{-5}atm-m^3/mole
Half lives-$t_{1/2}$		
1-Hydrolysis as a function of Ph	N/A	Can not be estimated
2-Photolysis (Atmospheric OH Rate Constant)	Half-life = 0.277 days	Atmospheric Oxidation Rate Constant = 37.2E-12 cm^3/molecule-sec Half-Life = 3.44 hrs
(Atmosph. Oxidation, Ozone)	NA	Can not be estimated
Biodegradability		
BIOWIN1	0.6894	0.69 (Biodegrades fast)
BIOWIN2	0.7823	0.78 (biodegrades fast)
BIOWIN3 (Ultimate biodegradation)	2.9291	2.93 (weeks)
BIOWIN4 (Primary Biodegradation)	3.6714	3.67 (Days)
BIOWIN5	0.3984	0.39 (not readily degradable)
BIOWIN6	0.3651	0.37 (not readily degradable)
BIOWIN (Ready Biodegradability Prediction)		0.78 (Does not Biodegrade fast)
Multicase (Ready Biodegradability Prediction)	EQU not inside model domain	No
Environmental Partitioning		
(MacKay, (III))	Mass Amount (percent) Air 1.46 Water 53 Soil 45.4 Sediment 0.094	Level III Fugacity Model: Mass Amount (percent) / Half-Life (hr) Air 1.23 / 6.64 Water 45.7 / 360 Soil 53 / 720 Sediment 0.089 3.24e+003

Fish Acute toxicity to fish (96hrs LC_{50}) mol/l Long term toxicity (28days NOEC) mol/l	LC50(non polar)`=906.93 LC50(polar) = 195.87 (Bintein)  LC50(non polar)`=`314.97 LC50(polar) = 73.428 (Syracuse)	LC_{50} (96hrs) = 1045 mg/l ChV(30days)= 112 mg/l, where CHV is chronic toxicity value
Daphnia Acute toxicity to Daphnia (48hrs EC_{50}) mol/l Long term toxicity (21days NOEC) mol/l	Not reliable, outside model domain (multicase)	LC_{50} (48hrs) = 1036 mg/l
Algae Acute toxicity to Algae (72hrs EC_{50}) mol/l	Not reliable, outside model domain (multicase)	EC_{50} (96-hr) = 606 mg/l

Table5: Comparison between the results obtained from EPIWIN and Danish(Q)SAR and

Step 5: Assess your substance to identify whether it is PBT or vPvB

Is your substance persistent? (Degradation properties)

The assessment of persistence is based on the degradation (biotic and chemical) and half life data available. Where no measured environmental degradation data are available, the predicted one can be used as a screen to indicate persistence.

With regard to the chemical degradation, the predicted rate constant and estimated half-life for the reaction of hydroxyl radicals with Ethyl Xanthate in the atmosphere indicated that when Ethyl Xanthate is released to the atmosphere is likely to be **degraded** (not persistence) by this fate process. The PBT Profiler has estimated that Ethyl Xanthate is expected to be found predominantly in soil and its persistence estimate is based on its transformation in this medium. Its half-life in soil, 30 days, does not exceed the EU criteria of 120 days). As expected, this result is similar to EPIWIN v3.2 estimate for Level III Fugacity Model (since PBT profile uses EPIWINV3.2 for this). Therefore, Ethyl Xanthate is estimated not to be persistent in the environment.

With regard to the biotic degradation assessment, the ready biodegradability prediction can be used to determine if a substance meets the P criteria. BIOWIN v4.02 gives an overall prediction that the substance is **not readily biodegradable**. However, some degradation is expected to occur according to the models.

A As a conclusion, based on the degradation and half life data (measured or estimated by PBT profile and EPIWIN), Ethyl Xanthate is considered to meet the screening criteria for persistence.

Is your substance bioaccumlative?

The potential for bioaccumulation is assessed on the basis of BCF. No measured BCF data are available. The potential for bioaccumulation was therefore assessed on the basis of a calculated BCF.

Both BCFWIN v2.17 and multicase predict BCF of 3.16 and 1 respectively (<2000). Moreover, BCF estimate from PBT profiler is also in consistent with BIOWIN.

Based on the above estimates, Ethyl Xanthate is not expected to bioaccumulate in the food chain and therefore is not considered to meet the screening criteria for bioaccumulation.

Is your substance toxic to the environment organisms?

As seen above, no measured data are available on the ecotoxicity of Ethyl Xanthate Where no measured data are available, the predicted one can be used as a screen to indicate toxicity.

ECOSAR v0.99 predicts acute L(E)C_{50} values for fish and Daphnia; (LC_{50}(96h) of 1045 mg/l for fish and LC_{50}(48hrs) of 1036 mg/l for Daphnia). Chronic toxicity data for the same species were also predicted by this model. These values are clearly above 0.1mg/l. It is therefore considered reasonably to conclude that the EU criteria for toxicity are not met. This is in consistent with PBT profiler ecotoxicity estimate for Ethyl Xanthate.

In conclusion, based on the available data (measured and estimate) Ethyl Xanthate is not considered fulfilling the T screening criterion.

Is your chemical classified as potential PBT?

Based on the predictions data, the substance has been shown to be not readily biodegradable and therefore is persistent. Both the estimated and measured BCF for the substance in fish are far below 2000. Therefore the substance does not fulfil the B-criterion. The measured and estimated aquatic toxicity data for Ethyl Xanthate are clearly above 0.1mg/l, therefore the substance does not fulfil the T-criterion.

Therefore on the basis of the predictions data the substance should not be considered as a potential PBT. However the substance is considered to be a potential P.

What is the preferred environmental compartment of your chemical? (Environmental Distribution)

Adsorption:

According to Mackay level III predictions the soil is the preferred environmental compartment (53%) for Ethyl Xanthate. In addition, the estimated Koc value (1) suggests that Ethyl Xanthate is expected to have low mobility in soil.