

**Appendix B. Predicted Toxicity of the Degradates to Aquatic Organisms Using ECOSAR
Version 1.0**

Table B1. Summary of ECOSAR Results Estimated for the Degradates of Thiobencarb

Endpoint	Thiobencarb	4-chlorobenzoic acid	4-chlorobenzaldehyde	Thiobencarb sulfoxide	2-hydroxythiobencarb	4-chlorobenzylmethylsulfone	4-chlorobenzylmethylsulfoxide	Bencarb	Desethyl Thiobencarb
ECOSAR Class	Thiocarbamate, Mono	Neutral Organics-acid	Aldehydes, mono	Amide	Phenol, thiocarbamate, mono	Neutral Organics	Neutral Organics	Carbamate Ester	Thiocarbamate, Mono
96-Hr LC50 FW Fish (mg/L)	2.877	421.723	5.527	740.075	3.744 6.125	725.752	847.468	1.588	7.089
48-Hr LC50 Daphnid (mg/L)	3.623	256.768	7.417	237.168	2.254 9.446	366.123	420.213	1.514	12.008
NOAEL or ChV FW Fish (mg/L)	0.126	45.491 32.318	0.693	1.840	0.429, 0.008 0.297	71.890	83.293	0.053	0.360
Daphnid NOAEL or ChV (mg/L)	0.462	32.318	1.135	4.375	0.428 1.084	37.670	42.444	0.018	1.312
Green Algae 96-hr EC50 (mg/L)	0.391	152.688	12.955	3.129	9.033 1.261	125.301	136.706	106.679	1.276
96-Hr LC50 SW Fish (mg/L)	0.397	563.642	--	0.491	1.164	1068.433	1258.732	0.331	1.343
96-hr LC50 Mysid Shrimp (mg/L)	0.321	290.450	--		-- 0.625	1238.684	1571.988		0.694
NOAEL or ChV	0.633	82.765	0.624		4.168 1.191	68.559	74.864	0.014	1.301

SW Fish (mg/L)									
NOAEL or ChV Mysid Shrimp (mg/L)	0.032	21.527			0.139	133.848	175.840		0.222

Thiobencarb

SMILES : CCN(CC)C(=O)SCc1ccc(CL)cc1

CHEM :

CAS Num:

ChemID1:

ChemID2:

ChemID3:

MOL FOR: C12 H16 CL1 N1 O1 S1

MOL WT : 257.78

Log Kow: 3.90 (KowWin estimate)

Melt Pt:

Wat Sol: 28 mg/L (experimental database)

ECOSAR v1.00 Class(es) Found

Thiocarbamates, Mono

		Predicted		
ECOSAR Class	Organism	Duration	End Pt	mg/L (ppm)
=====				
=====				
Thiocarbamates, Mono	: Fish	96-hr	LC50	2.877
Thiocarbamates, Mono	: Daphnid	48-hr	LC50	3.623
Thiocarbamates, Mono	: Green Algae	96-hr	EC50	0.792
Thiocarbamates, Mono	: Fish		ChV	0.126 !
Thiocarbamates, Mono	: Daphnid		ChV	0.462 !
Thiocarbamates, Mono	: Green Algae		ChV	0.391
Thiocarbamates, Mono	: Fish (SW)	96-hr	LC50	0.397
Thiocarbamates, Mono	: Mysid Shrimp (SW)	96-hr	LC50	0.321
Thiocarbamates, Mono	: Fish (SW)		ChV	0.633 !
Thiocarbamates, Mono	: Mysid Shrimp (SW)		ChV	0.032 !

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Neutral Organic SAR	: Fish	96-hr	LC50	4.927
(Baseline Toxicity)	: Daphnid	48-hr	LC50	3.576
	: Green Algae	96-hr	EC50	3.358
	: Fish		ChV	0.449
	: Daphnid		ChV	0.462
	: Green Algae		ChV	1.718

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.

Note: ! = exclamation designates: The toxicity value was determined from a predicted SAR using established acute-to-chronic ratios and ECOSAR regression techniques which are documented in the supporting Technical Reference Manual. When possible, this toxicity value should be considered in a weight of evidence approach.

Thiocarbamates, Mono :

For All Acute and Chronic Toxicity Values: If the log Kow of the chemical is greater than the value listed below, or if the compound is solid and the LC50, EC50 or ChV exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

ECOSAR v1.00 SAR Limitations:

Maximum LogKow: 5.0 (Fish 96-hr LC50, Daphnid LC50)

Maximum LogKow: 6.4 (Green Algae EC50)

Maximum LogKow: 8.0 (ChV)

Maximum LogKow: 8.0 (Fish (SW) 96-hr LC50)

Maximum LogKow: 5.0 (Mysid Shrimp LC50)

Maximum Mol Wt: 1000

Baseline Toxicity SAR Limitations:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50)

Maximum LogKow: 6.4 (Green Algae EC50)

Maximum LogKow: 8.0 (ChV)

Maximum Mol Wt: 1000

Thiobencarb sulfoxide

SMILES : CCN(CC)S(=O)S(=O)Cc1ccc(CL)cc1

CHEM :

CAS Num:

ChemID1:

ChemID2:

ChemID3:

MOL FOR: C11 H16 CL1 N1 O2 S2

MOL WT : 293.83

Log Kow: 0.37 (KowWin estimate)

Melt Pt:

Wat Sol: 6478 mg/L (WskowWin estimate)

ECOSAR v1.00 Class(es) Found

Amides

ECOSAR Class	Organism	Predicted Duration	End Pt	mg/L (ppm)
Amides	: Fish	96-hr	LC50	740.075
Amides	: Daphnid	48-hr	LC50	237.168
Amides	: Green Algae	96-hr	EC50	1.840
Amides	: Fish		ChV	4.375
Amides	: Daphnid		ChV	3.129 !
Amides	: Green Algae		ChV	0.491

Neutral Organic SAR	: Fish	96-hr	LC50	5450.916
(Baseline Toxicity)	: Daphnid	48-hr	LC50	2581.948
	: Green Algae	96-hr	EC50	569.616
	: Fish		ChV	536.469
	: Daphnid		ChV	178.669
	: Green Algae		ChV	153.004

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.

Note: ! = exclamation designates: The toxicity value was determined from a predicted SAR using established acute-to-chronic ratios and ECOSAR regression techniques which are documented in the supporting Technical Reference Manual. When possible, this toxicity value should be considered in a weight of evidence approach.

Amides :

No limitations known at this time.

ECOSAR v1.00 SAR Limitations:

Maximum LogKow: >8.5 (LC50)
Maximum LogKow: >8.0 (EC50,ChV)
Maximum Mol Wt: 1000

Baseline Toxicity SAR Limitations:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50)

Maximum LogKow: 6.4 (Green Algae EC50)

Maximum LogKow: 8.0 (ChV)

Maximum Mol Wt: 1000

2-hydroxythiobencarb

SMILES : CCN(CC)C(=O)SCc1ccc(CL)cc1O

CHEM :

CAS Num:

ChemID1:

ChemID2:

ChemID3:

MOL FOR: C12 H16 CL1 N1 O2 S1

MOL WT : 273.78

Log Kow: 3.42 (KowWin estimate)

Melt Pt:

Wat Sol: 79.85 mg/L (WskowWin estimate)

ECOSAR v1.00 Class(es) Found

Phenols

Thiocarbamates, Mono

ECOSAR Class		Organism	Predicted		mg/L (ppm)
			Duration	End Pt	
=====					
=====					
Phenols	:	Fish	96-hr	LC50	3.744
Phenols	:	Fish	14-day	LC50	12.368
Phenols	:	Daphnid	48-hr	LC50	2.254
Phenols	:	Green Algae	96-hr	EC50	9.033
Phenols	:	Fish	30-day	ChV	0.429
Phenols	:	Fish	60-day	ChV	0.008
Phenols	:	Daphnid	21-day	ChV	0.428
Phenols	:	Green Algae		ChV	4.168
Phenols	:	Fish (SW)	96-hr	LC50	1.164
Phenols	:	Earthworm	14-day	LC50	66.993
Phenols	:	Lemna Gibba	7-day	EC50	2.002
Thiocarbamates, Mono	:	Fish	96-hr	LC50	6.125
Thiocarbamates, Mono	:	Daphnid	48-hr	LC50	9.446
Thiocarbamates, Mono	:	Green Algae	96-hr	EC50	1.261
Thiocarbamates, Mono	:	Fish		ChV	0.297 !
Thiocarbamates, Mono	:	Daphnid		ChV	1.084 !
Thiocarbamates, Mono	:	Green Algae		ChV	0.632
Thiocarbamates, Mono	:	Fish (SW)	96-hr	LC50	1.049
Thiocarbamates, Mono	:	Mysid Shrimp (SW)	96-hr	LC50	0.625
Thiocarbamates, Mono	:	Fish (SW)		ChV	1.191 !

Thiocarbamates, Mono : Mysid Shrimp (SW) ChV 0.139 !

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Neutral Organic SAR : Fish 96-hr LC50 13.339
(Baseline Toxicity) : Daphnid 48-hr LC50 9.135
: Green Algae 96-hr EC50 7.044
: Fish ChV 1.227
: Daphnid ChV 1.084
: Green Algae ChV 3.302

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.

Note: ! = exclamation designates: The toxicity value was determined from a predicted SAR using established acute-to-chronic ratios and ECOSAR regression techniques which are documented in the supporting Technical Reference Manual. When possible, this toxicity value should be considered in a weight of evidence approach.

Phenols:

For All Acute and Chronic Toxicity Values: If the log Kow of the chemical is greater than the value listed below, or if the compound is solid and the LC50, EC50 or ChV exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

ECOSAR v1.00 SAR Limitations:

Maximum LogKow: 7.0 (Fish 96-hr LC50, Daphnid LC50)
Maximum LogKow: 6.4 (Fish 14-day LC50, Earthworm, Lemna)
Maximum LogKow: 7.0 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)
Maximum LogKow: 5.0 (Fish (SW) 96-hr LC50, Mysid)
Maximum Mol Wt: 1000

Thiocarbamates, Mono :

For All Acute and Chronic Toxicity Values: If the log Kow of the chemical is greater than the value listed below, or if the compound is solid and the LC50, EC50 or ChV exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

ECOSAR v1.00 SAR Limitations:

Maximum LogKow: 5.0 (Fish 96-hr LC50, Daphnid LC50)

Maximum LogKow: 6.4 (Green Algae EC50)
 Maximum LogKow: 8.0 (ChV)
 Maximum LogKow: 8.0 (Fish (SW) 96-hr LC50)
 Maximum LogKow: 5.0 (Mysid Shrimp LC50)
 Maximum Mol Wt: 1000

Baseline Toxicity SAR Limitations:

 Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50)
 Maximum LogKow: 6.4 (Green Algae EC50)
 Maximum LogKow: 8.0 (ChV)
 Maximum Mol Wt: 1000

4-chlorobenzoic acid

SMILES : O=C(O)c1ccc(Cl)cc1

CHEM :

CAS Num:

ChemID1:

ChemID2:

ChemID3:

MOL FOR: C7 H5 CL1 O2

MOL WT : 156.57

Log Kow: 2.52 (KowWin estimate)

Melt Pt:

Wat Sol: 72 mg/L (experimental database)

ECOSAR v1.00 Class(es) Found

 Neutral Organics-acid

ECOSAR Class	Organism	Predicted		
		Duration	End Pt	mg/L (ppm)
=====	=====	=====	=====	=====
=====	=====	=====	=====	=====

--> Acid moiety found: Predicted values multiplied by 10

Neutral Organics-acid	: Fish	96-hr	LC50	421.723 *
Neutral Organics-acid	: Fish	14-day	LC50	429.991 *
Neutral Organics-acid	: Daphnid	48-hr	LC50	256.768 *
Neutral Organics-acid	: Green Algae	96-hr	EC50	152.688 *
Neutral Organics-acid	: Fish	30-day	ChV	45.491
Neutral Organics-acid	: Daphnid		ChV	32.318
Neutral Organics-acid	: Green Algae		ChV	63.617
Neutral Organics-acid	: Fish (SW)	96-hr	LC50	563.642 *
Neutral Organics-acid	: Mysid Shrimp	96-hr	LC50	290.450 *
Neutral Organics-acid	: Fish (SW)		ChV	82.765 *
Neutral Organics-acid	: Mysid Shrimp (SW)		ChV	21.527

Neutral Organics-acid : Earthworm 14-day LC50 2404.901 *

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.

Neutral Organics:

For Fish LC50 (96-h), Daphnid LC50, Mysid: If the log Kow is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

For Fish LC50 (14-day) and Earthworm LC50: If the log Kow is greater than 6.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

For Green Algae Acute Toxicity Values: If the log Kow of the chemical is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

For All Chronic Toxicity Values: If the log Kow of the chemical is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

ECOSAR v1.00 SAR Limitations:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50, Mysid LC50)
Maximum LogKow: 6.0 (Fish 14-day LC50; Earthworm LC50)
Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)
Maximum Mol Wt: 1000

4-chlorobenzaldehyde

SMILES : O=Cc1ccc(CL)cc1

CHEM :

CAS Num:

ChemID1:

ChemID2:

ChemID3:

MOL FOR: C7 H5 CL1 O1

MOL WT : 140.57

Log Kow: 2.35 (KowWin estimate)

Melt Pt:

Wat Sol: 1340 mg/L (WskowWin estimate)

ECOSAR v1.00 Class(es) Found

Aldehydes (Mono)

ECOSAR Class	Organism	Predicted Duration	End Pt	mg/L (ppm)
=====	=====	=====	=====	=====
=====	=====	=====	=====	=====
Aldehydes (Mono)	: Fish	96-hr	LC50	5.527
Aldehydes (Mono)	: Daphnid	48-hr	LC50	7.417
Aldehydes (Mono)	: Green Algae	96-hr	EC50	12.955
Aldehydes (Mono)	: Fish		ChV	0.693
Aldehydes (Mono)	: Daphnid		ChV	1.135 !
Aldehydes (Mono)	: Green Algae		ChV	4.589
Aldehydes (Mono)	: Fish (SW)	96-hr	LC50	5.322
Aldehydes (Mono)	: Fish (SW)		ChV	0.624 !
=====	=====	=====	=====	=====
=====	=====	=====	=====	=====
Neutral Organic SAR	: Fish	96-hr	LC50	54.256
(Baseline Toxicity)	: Daphnid	48-hr	LC50	32.679
	: Green Algae	96-hr	EC50	16.296
	: Fish		ChV	5.110
	: Daphnid		ChV	3.214
	: Green Algae		ChV	6.292

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.

Note: ! = exclamation designates: The toxicity value was determined from a predicted SAR using established acute-to-chronic ratios and ECOSAR regression techniques which are documented in the supporting Technical Reference Manual. When possible, this toxicity value should be considered in a weight of evidence approach.

Aldehydes (Mono):

For Fish and Daphnid Acute Toxicity Values: If the log Kow of the chemical is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

For Green Algae Acute Toxicity Values: If the log Kow of the chemical is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

For All Chronic Toxicity Values: If the log Kow of the chemical is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

ECOSAR v1.00 SAR Limitations:

 Maximum LogKow: 5.0 (LC50)
 Maximum LogKow: 6.4 (EC50)
 Maximum LogKow: 8.0 (ChV)
 Maximum Mol Wt: 1000

Baseline Toxicity SAR Limitations:

 Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50)
 Maximum LogKow: 6.4 (Green Algae EC50)
 Maximum LogKow: 8.0 (ChV)
 Maximum Mol Wt: 1000

4-chlorobenzylmethylsulfone

SMILES : CS(=O)(=O)Cc1ccc(CL)cc1

CHEM :

CAS Num:

ChemID1:

ChemID2:

ChemID3:

MOL FOR: C8 H9 CL1 O2 S1

MOL WT : 204.67

Log Kow: 1.25 (KowWin estimate)

Melt Pt:

Wat Sol: 3567 mg/L (WskowWin estimate)

ECOSAR v1.00 Class(es) Found

 Neutral Organics

ECOSAR Class	Organism	Predicted		
		Duration	End Pt	mg/L (ppm)
=====				
=====				
Neutral Organics	: Fish	96-hr	LC50	725.752
Neutral Organics	: Fish	14-day	LC50	724.962
Neutral Organics	: Daphnid	48-hr	LC50	366.123
Neutral Organics	: Green Algae	96-hr	EC50	125.301
Neutral Organics	: Fish	30-day	ChV	71.890
Neutral Organics	: Daphnid		ChV	37.670
Neutral Organics	: Green Algae		ChV	42.229
Neutral Organics	: Fish (SW)	96-hr	LC50	1068.433
Neutral Organics	: Mysid Shrimp	96-hr	LC50	1238.684
Neutral Organics	: Fish (SW)		ChV	68.559
Neutral Organics	: Mysid Shrimp (SW)		ChV	133.848

Neutral Organics : Earthworm 14-day LC50 425.968

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.

Neutral Organics:

For Fish LC50 (96-h), Daphnid LC50, Mysid: If the log Kow is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

For Fish LC50 (14-day) and Earthworm LC50: If the log Kow is greater than 6.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

For Green Algae Acute Toxicity Values: If the log Kow of the chemical is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

For All Chronic Toxicity Values: If the log Kow of the chemical is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

ECOSAR v1.00 SAR Limitations:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50, Mysid LC50)
Maximum LogKow: 6.0 (Fish 14-day LC50; Earthworm LC50)
Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)
Maximum Mol Wt: 1000

4-chlorobenzylmethylsulfoxide

SMILES : CS(=O)Cc1ccc(Cl)cc1

CHEM :

CAS Num:

ChemID1:

ChemID2:

ChemID3:

MOL FOR: C8 H9 CL1 O1 S1

MOL WT : 188.67

Log Kow: 1.13 (KowWin estimate)

Melt Pt:

Wat Sol: 5409 mg/L (WskowWin estimate)

ECOSAR v1.00 Class(es) Found

Neutral Organics

ECOSAR Class	Organism	Predicted Duration	End Pt	mg/L (ppm)
=====	=====	=====	=====	=====
Neutral Organics	: Fish	96-hr	LC50	847.468
Neutral Organics	: Fish	14-day	LC50	844.954
Neutral Organics	: Daphnid	48-hr	LC50	420.213
Neutral Organics	: Green Algae	96-hr	EC50	136.706
Neutral Organics	: Fish	30-day	ChV	83.293
Neutral Organics	: Daphnid		ChV	42.444
Neutral Organics	: Green Algae		ChV	45.186
Neutral Organics	: Fish (SW)	96-hr	LC50	1258.732
Neutral Organics	: Mysid Shrimp	96-hr	LC50	1571.988
Neutral Organics	: Fish (SW)		ChV	74.864
Neutral Organics	: Mysid Shrimp (SW)		ChV	175.840
Neutral Organics	: Earthworm	14-day	LC50	403.766

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.

Neutral Organics:

For Fish LC50 (96-h), Daphnid LC50, Mysid: If the log Kow is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

For Fish LC50 (14-day) and Earthworm LC50: If the log Kow is greater than 6.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

For Green Algae Acute Toxicity Values: If the log Kow of the chemical is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

For All Chronic Toxicity Values: If the log Kow of the chemical is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

ECOSAR v1.00 SAR Limitations:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50, Mysid LC50)
Maximum LogKow: 6.0 (Fish 14-day LC50; Earthworm LC50)
Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)
Maximum Mol Wt: 1000

Bencarb

SMILES : CCN(CC)C(=O)OCc1ccc(CL)cc1

CHEM :

CAS Num:

ChemID1:

ChemID2:

ChemID3:

MOL FOR: C12 H16 CL1 N1 O2

MOL WT : 241.72

Log Kow: 3.70 (KowWin estimate)

Melt Pt:

Wat Sol: 18.2 mg/L (WskowWin estimate)

ECOSAR v1.00 Class(es) Found

Carbamate Esters

ECOSAR Class	Organism	Predicted		
		Duration	End Pt	mg/L (ppm)
=====		=====		=====
=====				
Carbamate Esters	: Fish	96-hr	LC50	1.588
Carbamate Esters	: Fish (SW)	96-hr	LC50	0.331
Carbamate Esters	: Daphnid	48-hr	LC50	1.514
Carbamate Esters	: Green Algae	96-hr	EC50	106.679 *
Carbamate Esters	: Fish		ChV	0.053
Carbamate Esters	: Daphnid		ChV	0.018 !
Carbamate Esters	: Green Algae		ChV	23.649 *
Carbamate Esters	: Fish (SW)		ChV	0.014
Carbamate Esters	: Sea Urchin	48-hr	NEC	5.687

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Neutral Organic SAR	: Fish	96-hr	LC50	6.786
(Baseline Toxicity)	: Daphnid	48-hr	LC50	4.809
	: Green Algae	96-hr	EC50	4.165
	: Fish		ChV	0.620
	: Daphnid		ChV	0.600
	: Green Algae		ChV	2.056

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.

Note: ! = exclamation designates: The toxicity value was determined from a predicted SAR using established acute-to-chronic ratios and ECOSAR regression techniques which are documented in the supporting Technical

Reference Manual. When possible, this toxicity value should be considered in a weight of evidence approach.

Carbamate Esters :

For Fish and Daphnid Acute Toxicity Values: If the log Kow of the chemical is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

For Green Algae Acute Toxicity Values: If the log Kow of the chemical is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

For All Chronic Toxicity Values: If the log Kow of the chemical is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

ECOSAR v1.00 SAR Limitations:

Maximum LogKow: 5.0 (LC50)

Maximum LogKow: 6.4 (EC50)

Maximum LogKow: 8.0 (ChV)

Maximum Mol Wt: 1000

Baseline Toxicity SAR Limitations:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50)

Maximum LogKow: 6.4 (Green Algae EC50)

Maximum LogKow: 8.0 (ChV)

Maximum Mol Wt: 1000

Desethyl Thiobencarb

SMILES : CCNC(=O)SCc1ccc(CL)cc1

CHEM :

CAS Num:

ChemID1:

ChemID2:

ChemID3:

MOL FOR: C10 H12 CL1 N1 O1 S1

MOL WT : 229.73

Log Kow: 3.19 (KowWin estimate)

Melt Pt:

Wat Sol: 57.07 mg/L (WskowWin estimate)

ECOSAR v1.00 Class(es) Found

 Thiocarbamates, Mono

ECOSAR Class	Organism	Predicted		
		Duration	End Pt	mg/L (ppm)
=====				
=====				
Thiocarbamates, Mono	: Fish	96-hr	LC50	7.089
Thiocarbamates, Mono	: Daphnid	48-hr	LC50	12.008
Thiocarbamates, Mono	: Green Algae	96-hr	EC50	1.276
Thiocarbamates, Mono	: Fish		ChV	0.360 !
Thiocarbamates, Mono	: Daphnid		ChV	1.312 !
Thiocarbamates, Mono	: Green Algae		ChV	0.644
Thiocarbamates, Mono	: Fish (SW)	96-hr	LC50	1.343
Thiocarbamates, Mono	: Mysid Shrimp (SW)	96-hr	LC50	0.694
Thiocarbamates, Mono	: Fish (SW)		ChV	1.301 !
Thiocarbamates, Mono	: Mysid Shrimp (SW)		ChV	0.222 !

=====				
=====				
Neutral Organic SAR	: Fish	96-hr	LC50	17.253
(Baseline Toxicity)	: Daphnid	48-hr	LC50	11.503
	: Green Algae	96-hr	EC50	8.097
	: Fish		ChV	1.595
	: Daphnid		ChV	1.312
	: Green Algae		ChV	3.645

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.

Note: ! = exclamation designates: The toxicity value was determined from a predicted SAR using established acute-to-chronic ratios and ECOSAR regression techniques which are documented in the supporting Technical Reference Manual. When possible, this toxicity value should be considered in a weight of evidence approach.

Thiocarbamates, Mono :

 For All Acute and Chronic Toxicity Values: If the log Kow of the chemical is greater than the value listed below, or if the compound is solid and the LC50, EC50 or ChV exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

ECOSAR v1.00 SAR Limitations:

 Maximum LogKow: 5.0 (Fish 96-hr LC50, Daphnid LC50)
 Maximum LogKow: 6.4 (Green Algae EC50)

Maximum LogKow: 8.0 (ChV)
Maximum LogKow: 8.0 (Fish (SW) 96-hr LC50)
Maximum LogKow: 5.0 (Mysid Shrimp LC50)
Maximum Mol Wt: 1000

Baseline Toxicity SAR Limitations:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50)
Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)
Maximum Mol Wt: 1000