

APPENDIX E.

EPISuite Model Output

SMILES : S(CC)C(=O)N(CCC)CCC
 CHEM :
 CAS Num: 759-94-4
 ChemID1:
 ChemID2:
 ChemID3:
 MOL FOR: C9 H19 N1 O1 S1
 MOL WT : 189.32
 Log Kow: 3.02 (KowWin estimate)
 Melt Pt:
 Wat Sol: 375 mg/L (experimental database)

ECOSAR v1.00 Class(es) Found

 Thiocarbamates, Mono

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
=====	=====	=====	=====	=====
Thiocarbamates, Mono	: Fish	96-hr	LC50	7.546
Thiocarbamates, Mono	: Daphnid	48-hr	LC50	13.772
Thiocarbamates, Mono	: Green Algae	96-hr	EC50	1.220
Thiocarbamates, Mono	: Fish		ChV	0.398 !
Thiocarbamates, Mono	: Daphnid		ChV	1.448 !
Thiocarbamates, Mono	: Green Algae		ChV	0.619
Thiocarbamates, Mono	: Fish (SW)	96-hr	LC50	1.549
Thiocarbamates, Mono	: Mysid Shrimp (SW)	96-hr	LC50	0.715
Thiocarbamates, Mono	: Fish (SW)		ChV	1.323 !
Thiocarbamates, Mono	: Mysid Shrimp (SW)		ChV	0.306 !
=====	=====	=====	=====	=====
Neutral Organic SAR	: Fish	96-hr	LC50	20.062
(Baseline Toxicity)	: Daphnid	48-hr	LC50	13.093
	: Green Algae	96-hr	EC50	8.571
	: Fish		ChV	1.862
	: Daphnid		ChV	1.448
	: Green Algae		ChV	3.736

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

<http://www.epa.gov/oppt/exposure/pubs/episuted1.htm>
