ECOSAR Version 1.11 Results Page

```
SMILES : CCCCNP(=S)(N)NCNC(=O)N
CHEM   :
CAS Num:
ChemID1:
MOL FOR: C6 H18 N5 O1 P1 S1
MOL WT : 239.28
Log Kow: -1.694      (EPISuite Kowwin v1.68 Estimate)
Log Kow:             (User Entered)
Log Kow:             (PhysProp DB exp value - for comparison only)
Melt Pt:             (User Entered for Wat Sol estimate)
Melt Pt:             (deg C, PhysProp DB exp value for Wat Sol estimate)
Wat Sol: 3.711E+004 (mg/L, EPISuite WSKowwin v1.43 Estimate)
Wat Sol:             (User Entered)
Wat Sol:             (PhysProp DB exp value)
```

Values used to Generate ECOSAR Profile

```
Log Kow: -1.694      (EPISuite Kowwin v1.68 Estimate)
Wat Sol: 3.711E+004 (mg/L, EPISuite WSKowwin v1.43 Estimate)
```

ECOSAR v1.11 Class-specific Estimations

Substituted Ureas

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Substituted Ureas	: Fish	96-hr	LC50	75168.063 *
Substituted Ureas	: Daphnid	48-hr	LC50	99253.727 *
Substituted Ureas	: Green Algae	96-hr	EC50	11.050
Substituted Ureas	: Fish		ChV	732.930
Substituted Ureas	: Daphnid		ChV	1206.428
Substituted Ureas	: Green Algae		ChV	2.495
Substituted Ureas	: Fish (SW)	96-hr	LC50	1182.123
Substituted Ureas	: Mysid (SW)	96-hr	LC50	14474.629
Substituted Ureas	: Fish (SW)		ChV	26.751
Substituted Ureas	: Mysid (SW)		ChV	287.905
Neutral Organic SAR (Baseline Toxicity)	: Fish	96-hr	LC50	4.08e+005 *
	: Daphnid	48-hr	LC50	1.65e+005 *
	: Green Algae	96-hr	EC50	29967.453
	: Fish		ChV	26686.184
	: Daphnid		ChV	6220.908
	: Green Algae		ChV	3671.923

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect. If the effect level exceeds the water solubility by 10X, typically no effects at saturation (NES) are reported.

Class Specific LogKow Cut-Offs

If the log Kow of the chemical is greater than the endpoint specific cut-offs presented below, then no effects at saturation are expected for those endpoints.

Substituted Ureas:

Maximum LogKow: 5.0 (LC50)
Maximum LogKow: 6.4 (EC50)
Maximum LogKow: 8.0 (ChV)

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)

ECOSAR Version 1.11 Results Page

```
SMILES : NC(=O)NCN(CCC)P(=S)(N)N
CHEM   :
CAS Num:
ChemID1:
MOL FOR: C5 H16 N5 O1 P1 S1
MOL WT : 225.25
Log Kow: -2.185     (EPISuite Kowwin v1.68 Estimate)
Log Kow:            (User Entered)
Log Kow:            (PhysProp DB exp value - for comparison only)
Melt Pt:            (User Entered for Wat Sol estimate)
Melt Pt:            (deg C, PhysProp DB exp value for Wat Sol estimate)
Wat Sol: 1.161E+005 (mg/L, EPISuite WSKowwin v1.43 Estimate)
Wat Sol:            (User Entered)
Wat Sol:            (PhysProp DB exp value)
```

Values used to Generate ECOSAR Profile

```
Log Kow: -2.185     (EPISuite Kowwin v1.68 Estimate)
Wat Sol: 1.161E+005 (mg/L, EPISuite WSKowwin v1.43 Estimate)
```

ECOSAR v1.11 Class-specific Estimations

Substituted Ureas

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Substituted Ureas	Fish	96-hr	LC50	1.8e+005 *
Substituted Ureas	Daphnid	48-hr	LC50	2.79e+005 *
Substituted Ureas	Green Algae	96-hr	EC50	16.598
Substituted Ureas	Fish		ChV	1587.515
Substituted Ureas	Daphnid		ChV	2691.073
Substituted Ureas	Green Algae		ChV	3.389
Substituted Ureas	Fish (SW)	96-hr	LC50	1901.988
Substituted Ureas	Mysid (SW)	96-hr	LC50	35396.297
Substituted Ureas	Fish (SW)		ChV	39.119
Substituted Ureas	Mysid (SW)		ChV	826.304
Neutral Organic SAR (Baseline Toxicity)	Fish	96-hr	LC50	1.06e+006 *
	Daphnid	48-hr	LC50	4.09e+005 *
	Green Algae	96-hr	EC50	61709.641
	Fish		ChV	65747.328
	Daphnid		ChV	13619.921
	Green Algae		ChV	6835.047

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect. If the effect level exceeds the water solubility by 10X, typically no effects at saturation (NES) are reported.

Class Specific LogKow Cut-Offs

If the log Kow of the chemical is greater than the endpoint specific cut-offs presented below, then no effects at saturation are expected for those endpoints.

Substituted Ureas:

Maximum LogKow: 5.0 (LC50)
Maximum LogKow: 6.4 (EC50)
Maximum LogKow: 8.0 (ChV)

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)

ECOSAR Version 1.11 Results Page

```
SMILES : CCCCNP(=S)(N)NCNC(=O)NCNC(=O)N
CHEM   :
CAS Num:
ChemID1:
MOL FOR: C8 H22 N7 O2 P1 S1
MOL WT : 311.34
Log Kow: -3.150     (EPISuite Kowwin v1.68 Estimate)
Log Kow:            (User Entered)
Log Kow:            (PhysProp DB exp value - for comparison only)
Melt Pt:            (User Entered for Wat Sol estimate)
Melt Pt:            (deg C, PhysProp DB exp value for Wat Sol estimate)
Wat Sol: 2.527E+005 (mg/L, EPISuite WSKowwin v1.43 Estimate)
Wat Sol:            (User Entered)
Wat Sol:            (PhysProp DB exp value)
```

Values used to Generate ECOSAR Profile

```
Log Kow: -3.150     (EPISuite Kowwin v1.68 Estimate)
Wat Sol: 2.527E+005 (mg/L, EPISuite WSKowwin v1.43 Estimate)
```

ECOSAR v1.11 Class-specific Estimations

Substituted Ureas

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Substituted Ureas	Fish	96-hr	LC50	1.56e+006 *
Substituted Ureas	Daphnid	48-hr	LC50	3.32e+006 *
Substituted Ureas	Green Algae	96-hr	EC50	57.456
Substituted Ureas	Fish		ChV	11280.503
Substituted Ureas	Daphnid		ChV	20259.250
Substituted Ureas	Green Algae		ChV	9.625
Substituted Ureas	Fish (SW)	96-hr	LC50	7536.092
Substituted Ureas	Mysid (SW)	96-hr	LC50	3.19e+005 *
Substituted Ureas	Fish (SW)		ChV	128.466
Substituted Ureas	Mysid (SW)		ChV	10207.370
Neutral Organic SAR (Baseline Toxicity)	Fish	96-hr	LC50	1.08e+007 *
	Daphnid	48-hr	LC50	3.81e+006 *
	Green Algae	96-hr	EC50	3.97e+005 *
	Fish		ChV	6.02e+005 *
	Daphnid		ChV	98844.313
	Green Algae		ChV	36062.469

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect. If the effect level exceeds the water solubility by 10X, typically no effects at saturation (NES) are reported.

Class Specific LogKow Cut-Offs

If the log Kow of the chemical is greater than the endpoint specific cut-offs presented below, then no effects at saturation are expected for those endpoints.

Substituted Ureas:

Maximum LogKow: 5.0 (LC50)
Maximum LogKow: 6.4 (EC50)
Maximum LogKow: 8.0 (ChV)

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)

ECOSAR Version 1.11 Results Page

```
SMILES : CCCCNP(=S)(NCNC(=O)N)NCNC(=O)N
CHEM   :
CAS Num:
ChemID1:
MOL FOR: C8 H22 N7 O2 P1 S1
MOL WT : 311.34
Log Kow: -3.068      (EPISuite Kowwin v1.68 Estimate)
Log Kow:             (User Entered)
Log Kow:             (PhysProp DB exp value - for comparison only)
Melt Pt:             (User Entered for Wat Sol estimate)
Melt Pt:             (deg C, PhysProp DB exp value for Wat Sol estimate)
Wat Sol: 2.153E+005  (mg/L, EPISuite WSKowwin v1.43 Estimate)
Wat Sol:             (User Entered)
Wat Sol:             (PhysProp DB exp value)
```

Values used to Generate ECOSAR Profile

```
Log Kow: -3.068      (EPISuite Kowwin v1.68 Estimate)
Wat Sol: 2.153E+005  (mg/L, EPISuite WSKowwin v1.43 Estimate)
```

ECOSAR v1.11 Class-specific Estimations

Substituted Ureas

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Substituted Ureas	: Fish	96-hr	LC50	1.33e+006 *
Substituted Ureas	: Daphnid	48-hr	LC50	2.77e+006 *
Substituted Ureas	: Green Algae	96-hr	EC50	53.175
Substituted Ureas	: Fish		ChV	9825.274
Substituted Ureas	: Daphnid		ChV	17559.945
Substituted Ureas	: Green Algae		ChV	9.058
Substituted Ureas	: Fish (SW)	96-hr	LC50	6895.448
Substituted Ureas	: Mysid (SW)	96-hr	LC50	2.73e+005 *
Substituted Ureas	: Fish (SW)		ChV	119.422
Substituted Ureas	: Mysid (SW)		ChV	8485.347
Neutral Organic SAR (Baseline Toxicity)	: Fish	96-hr	LC50	9.12e+006 *
	: Daphnid	48-hr	LC50	3.24e+006 *
	: Green Algae	96-hr	EC50	3.49e+005 *
	: Fish		ChV	5.13e+005 *
	: Daphnid		ChV	85939.852
	: Green Algae		ChV	32209.154

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect. If the effect level exceeds the water solubility by 10X, typically no effects at saturation (NES) are reported.

Class Specific LogKow Cut-Offs

If the log Kow of the chemical is greater than the endpoint specific cut-offs presented below, then no effects at saturation are expected for those endpoints.

Substituted Ureas:

Maximum LogKow: 5.0 (LC50)
Maximum LogKow: 6.4 (EC50)
Maximum LogKow: 8.0 (ChV)

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)

ECOSAR Version 1.11 Results Page

```
SMILES : CCCCN(CNC(=O)N)P(=S)(N)NCNC(=O)N
CHEM   :
CAS Num:
ChemID1:
MOL FOR: C8 H22 N7 O2 P1 S1
MOL WT : 311.34
Log Kow: -3.068      (EPISuite Kowwin v1.68 Estimate)
Log Kow:             (User Entered)
Log Kow:             (PhysProp DB exp value - for comparison only)
Melt Pt:             (User Entered for Wat Sol estimate)
Melt Pt:             (deg C, PhysProp DB exp value for Wat Sol estimate)
Wat Sol: 2.153E+005 (mg/L, EPISuite WSKowwin v1.43 Estimate)
Wat Sol:             (User Entered)
Wat Sol:             (PhysProp DB exp value)
```

Values used to Generate ECOSAR Profile

```
Log Kow: -3.068      (EPISuite Kowwin v1.68 Estimate)
Wat Sol: 2.153E+005 (mg/L, EPISuite WSKowwin v1.43 Estimate)
```

ECOSAR v1.11 Class-specific Estimations

Substituted Ureas

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Substituted Ureas	Fish	96-hr	LC50	1.33e+006 *
Substituted Ureas	Daphnid	48-hr	LC50	2.77e+006 *
Substituted Ureas	Green Algae	96-hr	EC50	53.175
Substituted Ureas	Fish		ChV	9825.274
Substituted Ureas	Daphnid		ChV	17559.945
Substituted Ureas	Green Algae		ChV	9.058
Substituted Ureas	Fish (SW)	96-hr	LC50	6895.448
Substituted Ureas	Mysid (SW)	96-hr	LC50	2.73e+005 *
Substituted Ureas	Fish (SW)		ChV	119.422
Substituted Ureas	Mysid (SW)		ChV	8485.347
Neutral Organic SAR (Baseline Toxicity)	Fish	96-hr	LC50	9.12e+006 *
	Daphnid	48-hr	LC50	3.24e+006 *
	Green Algae	96-hr	EC50	3.49e+005 *
	Fish		ChV	5.13e+005 *
	Daphnid		ChV	85939.852
	Green Algae		ChV	32209.154

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect. If the effect level exceeds the water solubility by 10X, typically no effects at saturation (NES) are reported.

Class Specific LogKow Cut-Offs

If the log Kow of the chemical is greater than the endpoint specific cut-offs presented below, then no effects at saturation are expected for those endpoints.

Substituted Ureas:

Maximum LogKow: 5.0 (LC50)
Maximum LogKow: 6.4 (EC50)
Maximum LogKow: 8.0 (ChV)

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)

ECOSAR Version 1.11 Results Page

```
SMILES : CCCCNP(=S)(N)NCNP(=S)(N)NCCCC
CHEM   :
CAS Num:
ChemID1:
MOL FOR: C9 H28 N6 P2 S2
MOL WT : 346.43
Log Kow: -0.376      (EPISuite Kowwin v1.68 Estimate)
Log Kow:             (User Entered)
Log Kow:             (PhysProp DB exp value - for comparison only)
Melt Pt:             (User Entered for Wat Sol estimate)
Melt Pt:             (deg C, PhysProp DB exp value for Wat Sol estimate)
Wat Sol: 1.364E+004 (mg/L, EPISuite WSKowwin v1.43 Estimate)
Wat Sol:             (User Entered)
Wat Sol:             (PhysProp DB exp value)
```

Values used to Generate ECOSAR Profile

```
Log Kow: -0.376      (EPISuite Kowwin v1.68 Estimate)
Wat Sol: 1.364E+004 (mg/L, EPISuite WSKowwin v1.43 Estimate)
```

ECOSAR v1.11 Class-specific Estimations

```
*****************************************************************************
| Not Related to an Existing ECOSAR Class Definition                        |
|                                                                           |
| Estimates provided below use the Neutral Organics QSAR equations which    |
| represent baseline toxicity potential (minimum toxicity) assuming a simple |
| non-polar narcosis model.  Without empirical data on structurally similar |
| chemicals, it is uncertain if this substance will present significantly   |
| higher toxicity above baseline estimates.                                 |
*****************************************************************************
```

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organics	: Fish	96-hr	LC50	38759.016 *
Neutral Organics	: Daphnid	48-hr	LC50	17671.889 *
Neutral Organics	: Green Algae	96-hr	EC50	5313.645
Neutral Organics	: Fish		ChV	2924.648
Neutral Organics	: Daphnid		ChV	935.811
Neutral Organics	: Green Algae		ChV	853.668
Neutral Organics	: Fish (SW)	96-hr	LC50	48105.457 *
Neutral Organics	: Mysid	96-hr	LC50	1.79e+005 *
Neutral Organics	: Fish (SW)		ChV	1223.487
Neutral Organics	: Mysid (SW)		ChV	31255.869 *
Neutral Organics	: Earthworm	14-day	LC50	1062.282

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect. If the effect level exceeds the water solubility by 10X, typically no effects at saturation (NES) are reported.

Class Specific LogKow Cut-Offs

If the log Kow of the chemical is greater than the endpoint specific cut-offs presented below, then no effects at saturation are expected for those endpoints.

Neutral Organics:

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