Oxycarboxin

Other names:	1,4-Oxathiin, 2,3-dihydro-5-carboxanilido-6-methyl-, 4,4-dioxide
	1,4-Oxathiin-3-carboxamide, 5,6-dihydro-2-methyl-N-phenyl-, 4,4-dioxide
	1,4-Oxathiin-3-carboxanilide, 5,6-dihydro-2-methyl-, 4,4-dioxide
	2,3-Dihydro-5-carboxanilido-6-methyl-1,4-oxathiin 4,4-dioxide
	2,3-Dihydro-6-methyl-5-phenylcarbamoyl-1,4-oxathiin-4,4-dioxide
	5,6-Dihydro-2-methyl-1,4-oxathiin-3-carboxanilide 4,4-dioxide
	5,6-Dihydro-2-methyl-3-carboxanilido-1,4-oxathiin-4,4-dioxid
	5,6-Dihydro-2-methyl-N-phenyl-1,4-oxathiin-3-carboxamide 4,4-dioxide
	Carboxin sulfone
	DCMOD
	DCMOO
	Dihydro-2-methyl-1,4-oxathiin-3-carboxanilide 4,4-dioxide
	Dioxide of vitavax
	F 461
	F 461 (Pesticide)
	NSC 2322673
	Oxathiin-3-carboxamide, 5,6-dihydro-2-methyl-N-phenyl-, 4,4-dioxide
	Oxathiin-3-carboxanilide, 5,6-dihydro-2-methyl-, 4,4-dioxide
	Oxicarboxin
	Oxycarboxine
	Oxykisvax
	Plant Wax
	Plantvax
	Plantvax 20
	Rendor
	Vitavax sulfone
	Vitavex
Inchi:	InChI=1S/C12H13NO4S/c1-9-11(18(15,16)8-7-17-9)12(14)13-10-5-3-2-4-6-10/h2-6H,7-8
InchiKey:	AMEKQAFGQBKLKX-UHFFFAOYSA-N
Formula:	C12H13NO4S
SMILES:	CC1=C(C(=O)Nc2ccccc2)S(=O)(=O)CCO1
Mol. weight [g/mol]:	267.30
CAS:	5259-88-1

Physical Properties

Property code	Value	Unit	Source

gf	-382.02	kJ/mol	Joback Method
hf	-586.05	kJ/mol	Joback Method
hfus	37.67	kJ/mol	Joback Method
hvap	82.26	kJ/mol	Joback Method
log10ws	-2.43		Aqueous Solubility Prediction Method
log10ws	-2.28		Estimated Solubility Method
logp	1.302		Crippen Method
mcvol	186.530	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
tb	691.80	K	Joback Method
tc	921.28	K	Joback Method
tf	403.24 ± 0.20	K	NIST Webbook
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.37	J/mol×K	691.80	Joback Method
cpg	505.71	J/mol×K	730.05	Joback Method
cpg	518.86	J/mol×K	768.29	Joback Method
cpg	530.87	J/mol×K	806.54	Joback Method
cpg	541.75	J/mol×K	844.79	Joback Method
cpg	551.57	J/mol×K	883.03	Joback Method
cpg	560.35	J/mol×K	921.28	Joback Method
hfust	26.66	kJ/mol	401.50	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5259881&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume