Carboxin

Other names:	1,4-Oxathiin, 2,3-dihydro-5-carboxanilido-6-methyl-
	1,4-Oxathiin-3-carboxamide, 5,6-dihydro-2-methyl-N-phenyl-
	1,4-Oxathiin-3-carboxanilide, 5,6-dihydro-2-methyl-
	2,3-Dihydro-5-carboxanilido-6-methyl-1,4-oxathiin
	2,3-Dihydro-6-methyl-1,4-oxathiin-5-carboxanilide
	5,6-Dihydro-2-methyl-1,4-oxathiin-3-carboxanilide
	5,6-Dihydro-2-methyl-3-carboxanilido-1,4-oxathiin
	5,6-Dihydro-2-methyl-N-phenyl-1,4-oxathiin-3-carboxamide
	5,6-Dihydro-2-methyl-N-phenyl-1,4-oxathin-3-carboxanilide (carboxin)
	5-Carboxanilido-2,3-dihydro-6-methyl-1,4-oxathiin
	Carbathiin
	Carboxine
	D 735
	DCMO
	DMOC
	F 735
	Flo pro v seed protectant
	Kemikar
	Kisvax
	NSC 263492
	Oxatin
	V 4X
	Vitaflo 250
	Vitavax
	Vitavax 100
	Vitavax 735D
	Vitavax 75W
Inchi:	InChI=1S/C12H13NO2S/c1-9-11(16-8-7-15-9)12(14)13-10-5-3-2-4-6-10/h2-6H,7-8H2,1H
InchiKey:	GYSSRZJIHXQEHQ-UHFFFAOYSA-N
Formula:	C12H13NO2S
SMILES:	CC1=C(C(=O)Nc2ccccc2)SCCO1
Mol. weight [g/mol]:	235.30
CAS:	5234-68-4

Physical Properties

Property code	Value	Unit	Source

gf	119.64	kJ/mol	Joback Method
hf	-90.83	kJ/mol	Joback Method
hfus	30.42	kJ/mol	Joback Method
hvap	70.44	kJ/mol	Joback Method
log10ws	-3.14		Estimated Solubility Method
log10ws	-3.14		Aqueous Solubility Prediction Method
logp	2.620		Crippen Method
mcvol	174.790	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
rinpol	2211.00		NIST Webbook
rinpol	2211.00		NIST Webbook
rinpol	2211.00		NIST Webbook
tb	712.80	K	Joback Method
tc	969.26	K	Joback Method
tf	364.65	K	Aqueous Solubility Prediction Method
tf	364.64 ± 0.20	K	NIST Webbook
tf	371.00 ± 0.20	K	NIST Webbook
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.80	J/mol×K	712.80	Joback Method
cpg	472.21	J/mol×K	755.54	Joback Method
cpg	485.36	J/mol×K	798.29	Joback Method
cpg	497.34	J/mol×K	841.03	Joback Method
cpg	508.20	J/mol×K	883.77	Joback Method
cpg	518.02	J/mol×K	926.51	Joback Method
cpg	526.88	J/mol×K	969.26	Joback Method
hfust	28.19	kJ/mol	229.50	NIST Webbook

Sources

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=C5234684&Units=SI

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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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