Thiophanate

Other names:	Carbamic acid, [1,2-phenylenebis(iminocarbonothioyl)]bis-, diethyl ester
	Allophanic acid, 4,4'-o-phenylenebis[3-thio-, diethyl ester
	BAS 3220
	Cercobin
	Enovit
	Ethyl thiophanate
	NF 35
	NF 35, Fungicide
	PELT
	Thiofanate
	Thiophanat (German)
	Thiophanate ethyl
	Topsin
	Topsin NF 35
	1,2-Bis(3-ethoxycarbonyl-2-thioureido)benzene
	1,2-Bis[3-(ethoxycarbonyl)thioureido]benzene
	Cleary's 3336
	Diethyl 4,4'-o-phenylene-bis(3-thioallophanate)
	Thiophanat
	4,4'-o-Phenylenebis(ethyl 3-thioallophanate)
	Nemafax
	NSC 170810
	Pelt (pesticide)
	Topsin E
	Cleary 3336
Inchi:	InChI=1S/C14H18N4O4S2/c1-3-21-13(19)17-11(23)15-9-7-5-6-8-10(9)16-12(24)18-14(2(
InchiKey:	YFNCATAIYKQPOO-UHFFFAOYSA-N
Formula:	C14H18N4O4S2
SMILES:	CCOC(=O)NC(=S)Nc1ccccc1NC(=S)NC(=O)OCC
Mol. weight [g/mol]:	370.45
CAS:	23564-06-9

Physical Properties

Property code	Value	Unit	Source
gf	293.62	kJ/mol	Joback Method
hf	-89.95	kJ/mol	Joback Method

hfus	60.84	kJ/mol	Joback Method
hvap	107.21	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	2.572		Crippen Method
mcvol	263.260	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
tb	1044.72	K	Joback Method
tc	1289.21	K	Joback Method
tf	709.98	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	783.80	J/mol×K	1044.72	Joback Method
cpg	793.56	J/mol×K	1085.47	Joback Method
cpg	802.86	J/mol×K	1126.22	Joback Method
cpg	811.82	J/mol×K	1166.96	Joback Method
cpg	820.56	J/mol×K	1207.71	Joback Method
cpg	829.19	J/mol×K	1248.46	Joback Method
cpg	837.82	J/mol×K	1289.21	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C23564069&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

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