Thiofanox

Other names:	2-Butanone, 3,3-dimethyl-1-(methylthio)-, O-[(methylamino)carbonyl]oxime
	3,3-Dimethyl-1-(Methylthio)-2-butanone O-[(methylamino)carbonyl]oxime
	3,3-Dimethyl-1-(methylthio)-2-butanone O-(methylcarbamoyl)oxime
	3,3-dimethyl-1-(methylthio)butanone-O-(N-methylcarbamoyl)oxime
	DS 15647
	Dacamox
	Diamond shamrock DS-15647
	ENT 27851
	Rcra waste number P045
	Thiofanocarb
Inchi:	InChI=1S/C9H18N2O2S/c1-9(2,3)7(6-14-5)11-13-8(12)10-4/h6H2,1-5H3,(H,10,12)
InchiKey:	FZSVSABTBYGOQH-UHFFFAOYSA-N
Formula:	C9H18N2O2S
SMILES:	CNC(=O)ON=C(CSC)C(C)(C)C
Mol. weight [g/mol]:	218.32
CAS:	39196-18-4

Physical Properties

Property code	Value	Unit	Source
hf	-314.87	kJ/mol	Joback Method
hvap	60.14	kJ/mol	Joback Method
log10ws	-1.62		Aqueous Solubility Prediction Method
log10ws	-1.62		Estimated Solubility Method
logp	2.107		Crippen Method
mcvol	177.120	ml/mol	McGowan Method
pc	2295.91	kPa	Joback Method
rinpol	1274.00		NIST Webbook
rinpol	1279.00		NIST Webbook
tb	673.89	K	Joback Method
tc	895.18	K	Joback Method
tf	331.11 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	19.83	kJ/mol	330.20	NIST Webbook
hsubt	94.00 ± 6.00	kJ/mol	313.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39196184&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
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

hf:	Enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation 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