Butocarboxim

Other names:	2-Butanone, 3-(methylthio)-, O-[(methylamino)carbonyl]oxime
	2-Butanone, 3-(methylthio)-, O-(N-methylcarbamoyl)oxime
	Afiline
	Butocarboxime
	CO 755
	Drawin 755
	3-(Methylthio)-2-butanone O-((methylamino)carbonyl)oxime
	3-(Methylthio)butanone O-methylcarbamoyloxime
	3-(Methylthio)-2-butanone O-(methylcarbamoyl)oxime
	3-(Methylthio)-O-((methylamino)carbonyl)oxime-2-butanone
	2-Methylthio-O-(N-methylcarbamoyl)-butanonoxim-3
	2-(([(Methylamino)carbonyl]oxy)imino)-3-(methylsulfanyl)butane
Inchi:	InChI=1S/C7H14N2O2S/c1-5(6(2)12-4)9-11-7(10)8-3/h6H,1-4H3,(H,8,10)
InchiKey:	SFNPDDSJBGRXLW-UHFFFAOYSA-N
Formula:	C7H14N2O2S
SMILES:	CNC(=O)ON=C(C)C(C)SC
Mol. weight [g/mol]:	190.26
CAS:	34681-10-2

Physical Properties

Property code	Value	Unit	Source
hf	-270.12	kJ/mol	Joback Method
hvap	56.59	kJ/mol	Joback Method
log10ws	-1.93		Crippen Method
logp	1.470		Crippen Method
mcvol	148.940	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
rinpol	1550.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1571.00		NIST Webbook
tb	630.92	K	Joback Method
tc	852.06	K	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34681102&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature