2,3-Butanedione oxime thiosemicarbazone

Inchi: InChI=1S/C5H10N4OS/c1-3(4(2)9-10)7-8-5(6)11/h10H,1-2H3,(H3,6,8,11)/b7-3-,9-4+
InchiKey: JYFXRMZMTBRMHZ-CITSBAIRSA-N
Formula: C5H10N4OS
SMILES: CC(=NO)C(C)=NNC(N)=S
Mol. weight [g/mol]: 174.22
CAS: 5012-80-6

Physical Properties

Property code	Value	Unit	Source
hf	79.86	kJ/mol	Joback Method
hvap	74.00	kJ/mol	Joback Method
log10ws	-0.86		Crippen Method
logp	0.046		Crippen Method
mcvol	130.550	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
tb	751.84	K	Joback Method
tc	983.26	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=C5012806&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature