Butoxycarboxim

Inchi: InChI=1S/C7H14N2O4S/c1-5(6(2)14(4,11)12)9-13-7(10)8-3/h6H,1-4H3,(H,8,10)/b9-5+
InchiKey: CTJBHIROCMPUKL-WEVVVXLNSA-N
Formula: C7H14N2O4S
SMILES: CNC(=O)ON=C(C)C(C)S(C)(=O)=O
Mol. weight [g/mol]: 222.26
CAS: 34681-23-7

Physical Properties

Property code	Value	Unit	Source
hf	-765.34	kJ/mol	Joback Method
hvap	68.41	kJ/mol	Joback Method
log10ws	-0.88		Crippen Method
logp	0.151		Crippen Method
mcvol	160.680	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
rinpol	1400.00		NIST Webbook
rinpol	1419.00		NIST Webbook
tb	609.92	K	Joback Method
tc	807.36	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C34681237&Units=SI

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