Methyl 2-isothiocyanato-3-methylbutyrate

Inchi: InChI=1S/C7H11NO2S/c1-5(2)6(8-4-11)7(9)10-3/h5-6H,1-3H3
InchiKey: MFTMQIVHQZBFTC-UHFFFAOYSA-N
Formula: C7H11NO2S
SMILES: COC(=O)C(N=C=S)C(C)C
Mol. weight [g/mol]: 173.23
CAS: 114877-91-7

Physical Properties

Property code	Value	Unit	Source
hf	-159.10	kJ/mol	Joback Method
hvap	50.00	kJ/mol	Joback Method
log10ws	-1.42		Crippen Method
logp	1.287		Crippen Method
mcvol	134.660	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
tb	580.92	K	Joback Method
tc	807.86	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C114877917&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

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