2-Isothiocyanato-3-methylpentanoic acid ethyl ester

Inchi: InChI=1S/C9H15NO2S/c1-4-7(3)8(10-6-13)9(11)12-5-2/h7-8H,4-5H2,1-3H3
InchiKey: MKMRESATFYSQFA-UHFFFAOYSA-N
Formula: C9H15NO2S
SMILES: CCOC(=O)C(N=C=S)C(C)CC
Mol. weight [g/mol]: 201.29

Physical Properties

Property code	Value	Unit	Source
hf	-200.38	kJ/mol	Joback Method
hvap	54.45	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.067		Crippen Method
mcvol	162.840	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	1381.40		NIST Webbook
tb	626.68	K	Joback Method
tc	845.39	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=R177210&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