2-Isothiocyanato-2-methylpropionic acid ethyl ester

Inchi: InChI=1S/C7H11NO2S/c1-4-10-6(9)7(2,3)8-5-11/h4H2,1-3H3
InchiKey: YMAIQXMMMHWWHA-UHFFFAOYSA-N
Formula: C7H11NO2S
SMILES: CCOC(=O)C(C)(C)N=C=S
Mol. weight [g/mol]: 173.23

Physical Properties

Property code	Value	Unit	Source
hf	-157.29	kJ/mol	Joback Method
hvap	49.48	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	1.431		Crippen Method
mcvol	134.660	ml/mol	McGowan Method
pc	3076.16	kPa	Joback Method
rinpol	1132.00		NIST Webbook
tb	578.57	K	Joback Method
tc	809.72	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=R177196&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