Methyl 3-isothiocyanatopropionate

Inchi: InChI=1S/C5H7NO2S/c1-8-5(7)2-3-6-4-9/h2-3H2,1H3
InchiKey: VLIJIUDWAKBKSO-UHFFFAOYSA-N
Formula: C5H7NO2S
SMILES: COC(=O)CCN=C=S
Mol. weight [g/mol]: 145.18
CAS: 18967-35-6

Physical Properties

Property code	Value	Unit	Source
hf	-107.26	kJ/mol	Joback Method
hvap	46.32	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	0.652		Crippen Method
mcvol	106.480	ml/mol	McGowan Method
pc	3763.78	kPa	Joback Method
tb	536.04	K	Joback Method
tc	761.37	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=C18967356&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature