Ethyl 2-isothiocyanatopropionate

Other names: 2-Isothiocyanato-propionic acid ethyl ester
Inchi: InChI=1S/C6H9NO2S/c1-3-9-6(8)5(2)7-4-10/h5H,3H2,1-2H3
InchiKey: ALJGYASQFZQQJX-UHFFFAOYSA-N
Formula: C6H9NO2S
SMILES: CCOC(=O)C(C)N=C=S
Mol. weight [g/mol]: 159.21
CAS: 39574-16-8

Physical Properties

Property code	Value	Unit	Source
hf	-133.18	kJ/mol	Joback Method
hvap	48.16	kJ/mol	Joback Method
log10ws	-1.24		Crippen Method
logp	1.041		Crippen Method
mcvol	120.570	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
rinpol	1141.80		NIST Webbook
tb	558.48	K	Joback Method
tc	784.71	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C39574168&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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