Ethyl 3-isothiocyanatopropionate

Inchi: InChI=1S/C6H9NO2S/c1-2-9-6(8)3-4-7-5-10/h2-4H2,1H3
InchiKey: UPTRONYNXNYITM-UHFFFAOYSA-N
Formula: C6H9NO2S
SMILES: CCOC(=O)CCN=C=S
Mol. weight [g/mol]: 159.21
CAS: 17126-62-4

Physical Properties

Property code	Value	Unit	Source
hf	-127.90	kJ/mol	Joback Method
hvap	48.55	kJ/mol	Joback Method
log10ws	-1.13		Crippen Method
logp	1.042		Crippen Method
mcvol	120.570	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
rinpol	1229.30		NIST Webbook
tb	558.92	K	Joback Method
tc	780.20	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17126624&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature