2-Isothiocyanato-hexanoic acid ethyl ester

Inchi: InChI=1S/C9H15NO2S/c1-3-5-6-8(10-7-13)9(11)12-4-2/h8H,3-6H2,1-2H3
InchiKey: VIIMESNYNGVWOV-UHFFFAOYSA-N
Formula: C9H15NO2S
SMILES: CCCCC(N=C=S)C(=O)OCC
Mol. weight [g/mol]: 201.29

Physical Properties

Property code	Value	Unit	Source
hf	-195.10	kJ/mol	Joback Method
hvap	54.84	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.211		Crippen Method
mcvol	162.840	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	1401.20		NIST Webbook
rinpol	1401.20		NIST Webbook
tb	627.12	K	Joback Method
tc	841.49	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R177250&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