2,6-diisothiocyanato-hexanoic acid ethyl ester

Inchi: InChI=1S/C10H14N2O2S2/c1-2-14-10(13)9(12-8-16)5-3-4-6-11-7-15/h9H,2-6H2,1H3
InchiKey: QJXQTXCTKSKWGP-UHFFFAOYSA-N
Formula: C10H14N2O2S2
SMILES: CCOC(=O)C(CCCCN=C=S)N=C=S
Mol. weight [g/mol]: 258.36

Physical Properties

Property code	Value	Unit	Source
hf	68.33	kJ/mol	Joback Method
hvap	67.50	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.294		Crippen Method
mcvol	194.660	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	1847.10		NIST Webbook
tb	795.95	K	Joback Method
tc	1037.46	K	Joback Method

Sources

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=R177181&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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