1,8-Octane diisothiocyanate

Inchi: InChI=1S/C10H16N2S2/c13-9-11-7-5-3-1-2-4-6-8-12-10-14/h1-8H2
InchiKey: LVGANCPXXODGKA-UHFFFAOYSA-N
Formula: C10H16N2S2
SMILES: S=C=NCCCCCCCCN=C=S
Mol. weight [g/mol]: 228.38
CAS: 56312-14-2

Physical Properties

Property code	Value	Unit	Source
hf	318.41	kJ/mol	Joback Method
hvap	58.73	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.533		Crippen Method
mcvol	187.220	ml/mol	McGowan Method
pc	2195.89	kPa	Joback Method
tb	720.10	K	Joback Method
tc	955.48	K	Joback Method

Sources

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=C56312142&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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