

Cyclododecyl isothiocyanate

Inchi: InChI=1S/C13H23NS/c15-12-14-13-10-8-6-4-2-1-3-5-7-9-11-13/h13H,1-11H2
InchiKey: VSCLPFIUOOLQJ-UHFFFAOYSA-N
Formula: C13H23NS
SMILES: S=C=NC1CCCCCCCCCCC1
Mol. weight [g/mol]: 225.39
CAS: 59037-64-8

Physical Properties

Property code	Value	Unit	Source
hf	-10.22	kJ/mol	Joback Method
hvap	56.43	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.763		Crippen Method
mcvol	200.900	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
tb	687.96	K	Joback Method
tc	963.24	K	Joback Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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=C59037648&Units=SI>

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

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