

Dodecyl isothiocyanate

Inchi: InChI=1S/C13H25NS/c1-2-3-4-5-6-7-8-9-10-11-12-14-13-15/h2-12H2,1H3
InchiKey: LPVQVNLMFKGGCH-UHFFFAOYSA-N
Formula: C13H25NS
SMILES: CCCCCCCCCCCN=C=S
Mol. weight [g/mol]: 227.41
CAS: 1072-32-8

Physical Properties

Property code	Value	Unit	Source
hf	-27.58	kJ/mol	Joback Method
hvap	54.97	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	5.010		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	1674.16	kPa	Joback Method
tb	642.79	K	Joback Method
tc	836.76	K	Joback Method

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1072328&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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