

Tetradecyl isothiocyanate

Inchi: InChI=1S/C15H29NS/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-16-15-17/h2-14H2,1H3
InchiKey: PMVOXLZEOLARED-UHFFFAOYSA-N
Formula: C15H29NS
SMILES: CCCCCCCCCCCCCCN=C=S
Mol. weight [g/mol]: 255.46
CAS: 3224-48-4

Physical Properties

Property code	Value	Unit	Source
hf	-68.86	kJ/mol	Joback Method
hvap	59.42	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.790		Crippen Method
mcpvol	239.940	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
tb	688.55	K	Joback Method
tc	878.89	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=C3224484&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/92-922-6/Tetradecyl-isothiocyanate.pdf>

Generated by Cheméo on 2024-04-26 05:24:38.021980712 +0000 UTC m=+16398326.942558054.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.