

4-Mercaptobutyl isothiocyanate

Inchi: InChI=1S/C5H9NS2/c7-4-2-1-3-6-5-8/h7H,1-4H2
InchiKey: NSHSQTFUNFUMRM-UHFFFAOYSA-N
Formula: C5H9NS2
SMILES: S=C=NCCCCS
Mol. weight [g/mol]: 147.26

Physical Properties

Property code	Value	Unit	Source
hf	176.02	kJ/mol	Joback Method
hvap	43.90	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.799		Crippen Method
mcvol	115.390	ml/mol	McGowan Method
pc	3848.31	kPa	Joback Method
rinsol	1290.00		NIST Webbook
rinsol	1290.00		NIST Webbook
tb	522.61	K	Joback Method
tc	763.54	K	Joback Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R586802&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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