

2-Hexane isothiocyanate

Inchi:	InChI=1S/C7H13NS/c1-3-4-5-7(2)8-6-9/h7H,3-5H2,1-2H3
InchiKey:	GCZWLZBNDSJSQF-UHFFFAOYSA-N
Formula:	C7H13NS
SMILES:	CCCCC(C)N=C=S
Mol. weight [g/mol]:	143.25
CAS:	5334-87-2

Physical Properties

Property code	Value	Unit	Source
hf	90.98	kJ/mol	Joback Method
hvap	41.23	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.668		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
tb	505.07	K	Joback Method
tc	721.13	K	Joback Method

Sources

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=C5334872&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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