

Cyclohexane, isothiocyanato-

Other names:	Cyclohexyl isothiocyanate Isothiocyanatocyclohexane Isothiocyanic acid, cyclohexyl ester Cyclohexyl isothiocyanate, isothiocyanato- Cyclohexyl-isothiocyanat Isothiocyanocyclohexane Cyclohexane isothiocyanate
Inchi:	InChI=1S/C7H11NS/c9-6-8-7-4-2-1-3-5-7/h7H,1-5H2
InchiKey:	MZSJGCPBOVTKHR-UHFFFAOYSA-N
Formula:	C7H11NS
SMILES:	S=C=NC1CCCCC1
Mol. weight [g/mol]:	141.23
CAS:	1122-82-3

Physical Properties

Property code	Value	Unit	Source
hf	150.58	kJ/mol	Joback Method
hvap	42.05	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.422		Crippen Method
mcvol	116.360	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
rinpol	1260.00		NIST Webbook
rinpol	1231.00		NIST Webbook
ripol	1670.00		NIST Webbook
ripol	1670.00		NIST Webbook
ripol	1666.00		NIST Webbook
ripol	1666.00		NIST Webbook
ripol	1660.00		NIST Webbook
ripol	1667.00		NIST Webbook
tb	525.06	K	Joback Method
tc	781.13	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=C1122823&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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