

Propane, 1-isothiocyanato-3-(methylthio)-

Other names:	3-Methylthiopropyl isothiocyanate Isothiocyanic acid, 3-(methylthio)propyl ester
Inchi:	InChI=1S/C5H9NS2/c1-8-4-2-3-6-5-7/h2-4H2,1H3
InchiKey:	LDKSCZJUIURGMW-UHFFFAOYSA-N
Formula:	C5H9NS2
SMILES:	CSCCCN=C=S
Mol. weight [g/mol]:	147.26
CAS:	505-79-3

Physical Properties

Property code	Value	Unit	Source
hf	179.41	kJ/mol	Joback Method
hvap	43.98	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.842		Crippen Method
mcvol	115.390	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
rinpol	1291.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1316.10		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1316.10		NIST Webbook
ripol	1979.00		NIST Webbook
ripol	1970.00		NIST Webbook
tb	528.53	K	Joback Method
tc	768.94	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=C505793&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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