1-Isothiocyanato-3-(methyldisulfanyl)propane

Inchi: InChI=1S/C5H9NS3/c1-8-9-4-2-3-6-5-7/h2-4H2,1H3
InchiKey: BIKPUHNMDVNATR-UHFFFAOYSA-N
Formula: C5H9NS3
SMILES: CSSCCCN=C=S
Mol. weight [g/mol]: 179.33

Physical Properties

Property code	Value	Unit	Source
hf	221.28	kJ/mol	Joback Method
hvap	50.80	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.490		Crippen Method
mcvol	131.740	ml/mol	McGowan Method
pc	3708.97	kPa	Joback Method
rinpol	1590.50		NIST Webbook
rinpol	1590.50		NIST Webbook
tb	597.31	K	Joback Method
tc	858.49	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=U414858&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature