4-Methylthiobutyl isothiocyanate

Other names: 1-isothiocyanato-4-(methylthio)-butane
Inchi: InChI=1S/C6H11NS2/c1-9-5-3-2-4-7-6-8/h2-5H2,1H3
InchiKey: IHQDGXUYTSZGOG-UHFFFAOYSA-N
Formula: C6H11NS2
SMILES: CSCCCCN=C=S
Mol. weight [g/mol]: 161.29
CAS: 4430-36-8

Physical Properties

Property code	Value	Unit	Source
hf	158.77	kJ/mol	Joback Method
hvap	46.21	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	2.232		Crippen Method
mcvol	129.480	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
rinpol	1432.00		NIST Webbook
rinpol	1436.60		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1383.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1403.00		NIST Webbook
ripol	2041.00		NIST Webbook
ripol	2041.00		NIST Webbook
ripol	2132.00		NIST Webbook
ripol	2135.00		NIST Webbook
tb	551.41	K	Joback Method
tc	787.06	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=C4430368&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