1-Isothiocyanato-6-(methylsulfinyl)hexane

Inchi: InChI=1S/C8H15NOS2/c1-12(10)7-5-3-2-4-6-9-8-11/h2-7H2,1H3
InchiKey: XQZVZULJKVALRI-UHFFFAOYSA-N
Formula: C8H15NOS2
SMILES: CS(=O)CCCCCCN=C=S
Mol. weight [g/mol]: 205.34
CAS: 4430-35-7

Physical Properties

Property code	Value	Unit	Source
hf	-130.12	kJ/mol	Joback Method
hvap	56.57	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	2.028		Crippen Method
mcvol	163.530	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpol	2009.40		NIST Webbook
rinpol	2009.40		NIST Webbook
tb	586.67	K	Joback Method
tc	799.93	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4430357&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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