

3-Thia-5-hexene-1-thiol

Inchi:	InChI=1S/C5H10S2/c1-2-4-7-5-3-6/h2,6H,1,3-5H2
InchiKey:	IUMUJLWECLSGI-UHFFFAOYSA-N
Formula:	C5H10S2
SMILES:	C=CCSCCS
Mol. weight [g/mol]:	134.26

Physical Properties

Property code	Value	Unit	Source
gf	141.57	kJ/mol	Joback Method
hf	59.25	kJ/mol	Joback Method
hfus	15.60	kJ/mol	Joback Method
hvap	39.61	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.835		Crippen Method
mvol	109.710	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
rinpol	1090.00		NIST Webbook
rinpol	1090.00		NIST Webbook
tb	442.12	K	Joback Method
tc	662.50	K	Joback Method
tf	215.21	K	Joback Method
vc	0.405	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.54	J/mol×K	442.12	Joback Method
cpg	206.64	J/mol×K	478.85	Joback Method
cpg	216.23	J/mol×K	515.58	Joback Method
cpg	225.32	J/mol×K	552.31	Joback Method
cpg	233.92	J/mol×K	589.04	Joback Method
cpg	242.04	J/mol×K	625.77	Joback Method
cpg	249.70	J/mol×K	662.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R156882&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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