5-Methyl-3-thia-1-hexanethiol

Inchi: InChI=1S/C6H14S2/c1-6(2)5-8-4-3-7/h6-7H,3-5H2,1-2H3
InchiKey: PLFYWXBVQAASLC-UHFFFAOYSA-N
Formula: C6H14S2
SMILES: CC(C)CSCCS
Mol. weight [g/mol]: 150.31

Physical Properties

Property code	Value	Unit	Source
gf	59.71	kJ/mol	Joback Method
hf	-92.10	kJ/mol	Joback Method
hfus	15.94	kJ/mol	Joback Method
hvap	42.12	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	2.305		Crippen Method
mcvol	128.100	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
rinpol	1166.00		NIST Webbook
tb	467.88	K	Joback Method
tc	685.33	K	Joback Method
tf	213.24	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.45	J/mol×K	467.88	Joback Method
cpg	265.08	J/mol×K	504.12	Joback Method
cpg	277.09	J/mol×K	540.36	Joback Method
cpg	288.51	J/mol×K	576.61	Joback Method
cpg	299.34	J/mol×K	612.85	Joback Method
cpg	309.60	J/mol×K	649.09	Joback Method
cpg	319.29	J/mol×K	685.33	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=R157414&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume