3-Thia-1-hexanethiol

Inchi: InChI=1S/C5H12S2/c1-2-4-7-5-3-6/h6H,2-5H2,1H3
InchiKey: ZTLMBCCGUMJDFH-UHFFFAOYSA-N
Formula: C5H12S2
SMILES: CCCSCCS
Mol. weight [g/mol]: 136.28

Physical Properties

Property code	Value	Unit	Source
gf	53.73	kJ/mol	Joback Method
hf	-66.18	kJ/mol	Joback Method
hfus	16.88	kJ/mol	Joback Method
hvap	40.28	kJ/mol	Joback Method
log10ws	-1.87		Crippen Method
logp	2.059		Crippen Method
mcvol	114.010	ml/mol	McGowan Method
pc	3824.55	kPa	Joback Method
rinpol	1111.00		NIST Webbook
rinpol	1111.00		NIST Webbook
tb	445.44	K	Joback Method
tc	660.82	K	Joback Method
tf	216.97	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.39	J/mol×K	445.44	Joback Method
cpg	223.30	J/mol×K	481.34	Joback Method
cpg	233.71	J/mol×K	517.23	Joback Method
cpg	243.64	J/mol×K	553.13	Joback Method
cpg	253.08	J/mol×K	589.03	Joback Method
cpg	262.05	J/mol×K	624.92	Joback Method
cpg	270.56	J/mol×K	660.82	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=R156817&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