5-Methyl-4-mercaptohexan-2-ol, # 1

Inchi: InChI=1S/C7H16OS/c1-5(2)7(9)4-6(3)8/h5-9H,4H2,1-3H3
InchiKey: RTGGPWJVXQMFRP-UHFFFAOYSA-N
Formula: C7H16OS
SMILES: CC(O)CC(S)C(C)C
Mol. weight [g/mol]: 148.27

Physical Properties

Property code	Value	Unit	Source
gf	-106.69	kJ/mol	Joback Method
hf	-317.40	kJ/mol	Joback Method
hfus	11.45	kJ/mol	Joback Method
hvap	53.43	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.712		Crippen Method
mcvol	131.710	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
rinpol	1097.00		NIST Webbook
rinpol	1097.00		NIST Webbook
tb	513.28	K	Joback Method
tc	703.28	K	Joback Method
tf	220.93	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.66	J/mol×K	513.28	Joback Method
cpg	308.57	J/mol×K	544.95	Joback Method
cpg	319.93	J/mol×K	576.61	Joback Method
cpg	330.74	J/mol×K	608.28	Joback Method
cpg	341.03	J/mol×K	639.94	Joback Method
cpg	350.81	J/mol×K	671.61	Joback Method
cpg	360.09	J/mol×K	703.28	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R603219&Units=SI

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