5-Methyl-4-mercapto-2-hexanone

Inchi: InChI=1S/C7H14OS/c1-5(2)7(9)4-6(3)8/h5,7,9H,4H2,1-3H3
InchiKey: UQBDDFZDCXIBHM-UHFFFAOYSA-N
Formula: C7H14OS
SMILES: CC(=O)CC(S)C(C)C
Mol. weight [g/mol]: 146.25

Physical Properties

Property code	Value	Unit	Source
gf	-96.35	kJ/mol	Joback Method
hf	-272.47	kJ/mol	Joback Method
hfus	12.48	kJ/mol	Joback Method
hvap	43.88	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.920		Crippen Method
mcvol	127.410	ml/mol	McGowan Method
pc	3276.53	kPa	Joback Method
rinpol	1069.00		NIST Webbook
tb	475.41	K	Joback Method
tc	682.94	K	Joback Method
tf	225.04	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.97	J/mol×K	475.41	Joback Method
cpg	275.68	J/mol×K	510.00	Joback Method
cpg	287.76	J/mol×K	544.59	Joback Method
cpg	299.23	J/mol×K	579.18	Joback Method
cpg	310.10	J/mol×K	613.77	Joback Method
cpg	320.39	J/mol×K	648.35	Joback Method
cpg	330.12	J/mol×K	682.94	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=R603204&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