2-Hexanone, 5-mercapto

Inchi: InChI=1S/C6H12OS/c1-5(7)3-4-6(2)8/h6,8H,3-4H2,1-2H3
InchiKey: GFUOWPYWXSTOFZ-UHFFFAOYSA-N
Formula: C6H12OS
SMILES: CC(=O)CCC(C)S
Mol. weight [g/mol]: 132.22

Physical Properties

Property code	Value	Unit	Source
gf	-102.33	kJ/mol	Joback Method
hf	-246.55	kJ/mol	Joback Method
hfus	13.41	kJ/mol	Joback Method
hvap	42.05	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.674		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
rinpol	993.00		NIST Webbook
rinpol	993.00		NIST Webbook
tb	452.97	K	Joback Method
tc	658.46	K	Joback Method
tf	228.77	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.01	J/mol×K	452.97	Joback Method
cpg	233.16	J/mol×K	487.22	Joback Method
cpg	243.77	J/mol×K	521.47	Joback Method
cpg	253.86	J/mol×K	555.71	Joback Method
cpg	263.44	J/mol×K	589.96	Joback Method
cpg	272.53	J/mol×K	624.21	Joback Method
cpg	281.15	J/mol×K	658.46	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=R90505&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