6-Mercapto-2-hexanone

Inchi: InChI=1S/C6H12OS/c1-6(7)4-2-3-5-8/h8H,2-5H2,1H3
InchiKey: QGQSMYRKYYEGHB-UHFFFAOYSA-N
Formula: C6H12OS
SMILES: CC(=O)CCCCS
Mol. weight [g/mol]: 132.22

Physical Properties

Property code	Value	Unit	Source
gf	-99.89	kJ/mol	Joback Method
hf	-241.27	kJ/mol	Joback Method
hfus	16.94	kJ/mol	Joback Method
hvap	42.43	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.675		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
pc	3598.56	kPa	Joback Method
rinpol	1014.00		NIST Webbook
rinpol	1014.00		NIST Webbook
tb	453.41	K	Joback Method
tc	654.16	K	Joback Method
tf	243.77	K	Joback Method
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.86	J/mol×K	453.41	Joback Method
cpg	232.66	J/mol×K	486.87	Joback Method
cpg	242.96	J/mol×K	520.33	Joback Method
cpg	252.77	J/mol×K	553.79	Joback Method
cpg	262.11	J/mol×K	587.25	Joback Method
cpg	270.99	J/mol×K	620.71	Joback Method
cpg	279.41	J/mol×K	654.16	Joback Method

Sources

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=R568775&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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