

5-Mercaptohexan-3-one

Inchi:	InChI=1S/C6H12OS/c1-3-6(7)4-5(2)8/h5,8H,3-4H2,1-2H3
InchiKey:	FVUILWCIRQEGGQ-UHFFFAOYSA-N
Formula:	C6H12OS
SMILES:	CCC(=O)CC(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	984.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	984.00		NIST Webbook
ripol	1487.00		NIST Webbook
ripol	1487.00		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=R282481&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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