

4-Mercapto-4-methyl-2-pentanone

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

Physical Properties

Property code	Value	Unit	Source
gf	-97.05	kJ/mol	Joback Method
hf	-250.02	kJ/mol	Joback Method
hfus	9.52	kJ/mol	Joback Method
hvap	41.14	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.674		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
rinpol	915.00		NIST Webbook
rinpol	942.00		NIST Webbook
rinpol	942.00		NIST Webbook
ripol	1383.00		NIST Webbook
ripol	1383.00		NIST Webbook
tb	450.18	K	Joback Method
tc	664.66	K	Joback Method
tf	246.19	K	Joback Method
vc	0.420	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.71	J/mol×K	450.18	Joback Method
cpg	236.73	J/mol×K	485.93	Joback Method
cpg	247.99	J/mol×K	521.67	Joback Method
cpg	258.56	J/mol×K	557.42	Joback Method
cpg	268.45	J/mol×K	593.17	Joback Method

cpg	277.70	J/mol×K	628.92	Joback Method
cpg	286.35	J/mol×K	664.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R602578&Units=SI
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

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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