2-Pentanone, 4-mercapto-4-methyl-

Other names:	4-Methyl-4-thiolpentan-2-one
	4-Methyl-4-sulfanyl-2-pentanone
	4-Mercapto-4-methyl-2-pentanone
	4-Mercapto-4-methyl-pentan-2-one
	4-Methyl-4-mercapto-2-pentanone
	4-Sulfanyl-4-methylpentan-2-one
	4-Sulphanyl-4-methylpentan-2-one
	4-methyl-4-sulfanylpentan-2-one
	4-Methyl-4-mercaptopentan-2-one
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
CAS:	19872-52-7

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	948.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	915.00		NIST Webbook

rinpol	940.00	NIST Webbook
rinpol	944.00	NIST Webbook
rinpol	944.00	NIST Webbook
rinpol	934.00	NIST Webbook
rinpol	942.00	NIST Webbook
rinpol	924.00	NIST Webbook
rinpol	937.00	NIST Webbook
rinpol	943.00	NIST Webbook
rinpol	942.00	NIST Webbook
rinpol	941.00	NIST Webbook
rinpol	968.00	NIST Webbook
rinpol	944.00	NIST Webbook
rinpol	942.00	NIST Webbook
ripol	1380.00	NIST Webbook
ripol	1366.00	NIST Webbook
ripol	1382.00	NIST Webbook
ripol	1381.00	NIST Webbook
ripol	1383.00	NIST Webbook
ripol	1380.00	NIST Webbook
ripol	1387.00	NIST Webbook
ripol	1382.00	NIST Webbook
ripol	1383.00	NIST Webbook
ripol	1381.00	NIST Webbook
ripol	1366.00	NIST Webbook
ripol	1374.00	NIST Webbook
ripol	1389.00	NIST Webbook
ripol	1380.00	NIST Webbook
ripol	1394.00	NIST Webbook
ripol	1397.00	NIST Webbook
ripol	1380.00	NIST Webbook
ripol	1384.00	NIST Webbook
ripol	1383.00	NIST Webbook
ripol	1391.00	NIST Webbook
ripol	1395.00	NIST Webbook
ripol	1383.00	NIST Webbook
ripol	1363.00	NIST Webbook
ripol	1381.00	NIST Webbook
ripol	1377.00	NIST Webbook
ripol	1386.00	NIST Webbook
ripol	1390.00	NIST Webbook
ripol	1373.00	NIST Webbook
ripol	1389.00	NIST Webbook
ripol	1395.00	NIST Webbook
ripol	1387.00	NIST Webbook

ripol	1382.00		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=C19872527&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