3-Mercapto-2-pentanone

Other names: 2-Pentanone, 3-mercapto-
3-mercapto-2-penanone
3-mercaptopentan-2-one
Inchi: InChI=1S/C5H10OS/c1-3-5(7)4(2)6/h5,7H,3H2,1-2H3
InchiKey: SZECUQRKLXRGSJ-UHFFFAOYSA-N
Formula: C5H10OS
SMILES: CCC(S)C(C)=O
Mol. weight [g/mol]: 118.20

Physical Properties

Property code	Value	Unit	Source
gf	-110.75	kJ/mol	Joback Method
hf	-225.91	kJ/mol	Joback Method
hfus	10.82	kJ/mol	Joback Method
hvap	39.82	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	1.284		Crippen Method
mcvol	99.230	ml/mol	McGowan Method
pc	4093.38	kPa	Joback Method
rinpol	913.00		NIST Webbook
rinpol	907.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	907.00		NIST Webbook
rinpol	907.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	899.00		NIST Webbook
rinpol	898.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	899.00		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	907.00		NIST Webbook

rinpol	897.00		NIST Webbook
rinpol	897.00		NIST Webbook
rinpol	907.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	903.00		NIST Webbook
rinpol	907.00		NIST Webbook
ripol	1363.00		NIST Webbook
ripol	1358.00		NIST Webbook
ripol	1360.00		NIST Webbook
ripol	1346.00		NIST Webbook
ripol	1347.00		NIST Webbook
ripol	1363.00		NIST Webbook
ripol	1358.00		NIST Webbook
ripol	1363.00		NIST Webbook
ripol	1346.00		NIST Webbook
ripol	1343.00		NIST Webbook
ripol	1347.00		NIST Webbook
ripol	1345.00		NIST Webbook
ripol	1347.00		NIST Webbook
ripol	1347.00		NIST Webbook
ripol	1347.00		NIST Webbook
ripol	1354.00		NIST Webbook
tb	430.09	K	Joback Method
tc	638.12	K	Joback Method
tf	217.50	K	Joback Method
vc	0.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.43	J/mol×K	430.09	Joback Method
cpg	193.22	J/mol×K	464.76	Joback Method
cpg	202.55	J/mol×K	499.43	Joback Method
cpg	211.43	J/mol×K	534.10	Joback Method
cpg	219.86	J/mol×K	568.78	Joback Method
cpg	227.86	J/mol×K	603.45	Joback Method
cpg	235.44	J/mol×K	638.12	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=C67633970&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