2-Cyclopenten-1-one, 2-methyl-

Other names: 2-Methyl-2-cyclopentenone
2-Methyl-2-cyclopenten-1-one
Inchi: InChI=1S/C6H8O/c1-5-3-2-4-6(5)7/h3H,2,4H2,1H3
InchiKey: ZSBWUNDRDHVNJL-UHFFFAOYSA-N
Formula: C6H8O
SMILES: CC1=CCCC1=O
Mol. weight [g/mol]: 96.13
CAS: 1120-73-6

Physical Properties

Property code	Value	Unit	Source
gf	-58.36	kJ/mol	Joback Method
hf	-177.74	kJ/mol	Joback Method
hfus	4.50	kJ/mol	Joback Method
hvap	34.72	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	1.296		Crippen Method
mcvol	81.810	ml/mol	McGowan Method
pc	4299.92	kPa	Joback Method
rinpol	905.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	901.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	907.60		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	903.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	896.00		NIST Webbook
rinpol	907.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	881.00		NIST Webbook

rinpol	915.00		NIST Webbook
rinpol	127.90		NIST Webbook
rinpol	896.00		NIST Webbook
ripol	1373.00		NIST Webbook
ripol	1367.00		NIST Webbook
ripol	1355.00		NIST Webbook
ripol	1397.00		NIST Webbook
ripol	1356.00		NIST Webbook
ripol	1356.00		NIST Webbook
ripol	1366.00		NIST Webbook
ripol	1355.00		NIST Webbook
ripol	1354.00		NIST Webbook
ripol	1366.00		NIST Webbook
ripol	1367.00		NIST Webbook
ripol	1366.00		NIST Webbook
ripol	1397.00		NIST Webbook
ripol	1397.00		NIST Webbook
ripol	1386.00		NIST Webbook
ripol	1381.00		NIST Webbook
ripol	1395.00		NIST Webbook
ripol	1357.00		NIST Webbook
ripol	1381.00		NIST Webbook
ripol	1368.00		NIST Webbook
ripol	1349.00		NIST Webbook
ripol	1367.00		NIST Webbook
ripol	1354.00		NIST Webbook
ripol	1353.00		NIST Webbook
ripol	1355.00		NIST Webbook
ripol	1371.00		NIST Webbook
ripol	1371.00		NIST Webbook
ripol	1355.00		NIST Webbook
ripol	1357.00		NIST Webbook
ripol	1355.00		NIST Webbook
ripol	1367.00		NIST Webbook
tb	432.70	K	NIST Webbook
tb	430.20	K	NIST Webbook
tc	650.56	K	Joback Method
tf	254.02	K	Joback Method
vc	0.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	151.47	J/mol×K	428.59	Joback Method
cpg	162.58	J/mol×K	465.59	Joback Method
cpg	173.22	J/mol×K	502.58	Joback Method
cpg	183.40	J/mol×K	539.58	Joback Method
cpg	193.10	J/mol×K	576.57	Joback Method
cpg	202.34	J/mol×K	613.57	Joback Method
cpg	211.11	J/mol×K	650.56	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=C1120736&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