2-Cyclopenten-1-one, 2,3-dimethyl-

Other names:	2,3-dimethyl-2-cyclopentenone
	2,3-Dimethylcyclopent-2-en-1-one
	Cyclopent-2-en-1-one, 2,3-dimethyl
	2,3-Dimethyl-2-cyclopenten-1-one
Inchi:	InChI=1S/C7H10O/c1-5-3-4-7(8)6(5)2/h3-4H2,1-2H3
InchiKey:	UZLQSPYGTUMKGS-UHFFFAOYSA-N
Formula:	C7H10O
SMILES:	CC1=C(C)C(=O)CC1
Mol. weight [g/mol]:	110.15
CAS:	1121-05-7

Physical Properties

Property code	Value	Unit	Source
gf	-59.57	kJ/mol	Joback Method
hf	-209.85	kJ/mol	Joback Method
hfus	6.70	kJ/mol	Joback Method
hvap	37.61	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.686		Crippen Method
mcvol	95.900	ml/mol	McGowan Method
pc	3736.23	kPa	Joback Method
rinpol	999.00		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1040.00		NIST Webbook
ripol	1523.00		NIST Webbook
ripol	1531.00		NIST Webbook
ripol	1530.00		NIST Webbook
ripol	1521.00		NIST Webbook
ripol	1521.00		NIST Webbook
ripol	1524.00		NIST Webbook

ripol	1535.00		NIST Webbook
ripol	1501.00		NIST Webbook
ripol	1524.00		NIST Webbook
ripol	1550.00		NIST Webbook
ripol	1573.00		NIST Webbook
ripol	1550.00		NIST Webbook
ripol	1582.00		NIST Webbook
ripol	1582.00		NIST Webbook
ripol	1535.00		NIST Webbook
ripol	1541.00		NIST Webbook
ripol	1535.00		NIST Webbook
tb	456.45	K	Joback Method
tc	676.77	K	Joback Method
tf	277.81	K	Joback Method
vc	0.362	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.88	J/mol×K	456.45	Joback Method
cpg	202.98	J/mol×K	493.17	Joback Method
cpg	214.61	J/mol×K	529.89	Joback Method
cpg	225.75	J/mol×K	566.61	Joback Method
cpg	236.40	J/mol×K	603.33	Joback Method
cpg	246.56	J/mol×K	640.05	Joback Method
cpg	256.22	J/mol×K	676.77	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1121057&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