2-Cyclopenten-1-one, 3-methyl-

Other names:	1-Methyl-1-cyclopenten-3-one
	1-methyl-2-cyclopenten-3-one
	3-Methyl-2-cyclopentenone
	3-methyl-2-cyclopenten-1-one
	3-methylcyclopent-2-enone
Inchi:	InChI=1S/C6H8O/c1-5-2-3-6(7)4-5/h4H,2-3H2,1H3
InchiKey:	CHCCBPDEADMNCI-UHFFFAOYSA-N
Formula:	C6H8O
SMILES:	CC1=CC(=O)CC1
Mol. weight [g/mol]:	96.13
CAS:	2758-18-1

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	923.00		NIST Webbook
rinpol	973.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	154.17		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	973.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	154.17		NIST Webbook
ripol	1506.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1507.00		NIST Webbook

ripol	1501.00		NIST Webbook
ripol	1513.00		NIST Webbook
ripol	1498.00		NIST Webbook
ripol	1513.00		NIST Webbook
tb	430.70	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	202.34	J/mol×K	613.57	Joback Method
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	211.11	J/mol×K	650.56	Joback Method
hvapt	52.40	kJ/mol	298.15	Energetic vs structural study of two biomass degradation derivatives: 2-Cyclopentenone and 3-methyl-2-cyclopentenone

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	347.20	K	2.00	NIST Webbook

Sources

Liquid-Liquid Equilibria for the Ternary Systems Water + 3-Methyl-2-cyclopentenone with Ethyl Acetate or Methyl tert-Butyl Ether at 298.2 K:	https://www.doi.org/10.1021/je0502492
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=C2758181&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Energetic vs structural study of two biomass degradation derivatives: 2-Cyclopentenone and 3-methyl-2-cyclopentenone:	https://www.doi.org/10.1016/j.jct.2019.01.012

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
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume