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

Other names:	Corylon
	Corylone
	Cycloten
	Cyclotene
	2-Hydroxy-1-methylcyclopenten-3-one
	2-Hydroxy-3-methyl-2-cyclopenten-1-one
	Maple lactone
	2-Hydroxy-3-methyl-2-cyclopentene-1-one
	2-Hydroxy-3-methylcyclopent-2-en-1-one
	3-Methyl-2-hydroxy-2-cyclopentenone
	3-Methylcyclopent-2-en-2-ol-1-one
	Cyclotene (odorant)
	NSC 133445
	2-Hydroxy-3-methyl-2-cyclopenten-1-one (Cyclotene)
	2-Hydroxy-3-methyl-2-cyclopentene-1-one(cyclotene)
	2-Hydroxy-3-methylcyclopentenone
	2-hydroxy-3-methyl-2-cyclopenten1-one (cycloten)
	Methylcyclopentenolone
	2-hydroxy-3-methyl-2-cyclopentenone
	3-Methyl-1,2-cyclopentanedione (cyclotene)
	2-hydroxy-3-methylcyclopent-2-enone
Inchi:	InChI=1S/C6H8O2/c1-4-2-3-5(7)6(4)8/h8H,2-3H2,1H3
InchiKey:	CFAKWWQIUFSQFU-UHFFFAOYSA-N
Formula:	C6H8O2
SMILES:	CC1=C(O)C(=O)CC1
Mol. weight [g/mol]:	112.13
CAS:	80-71-7

Physical Properties

Property code	Value	Unit	Source
gf	-204.81	kJ/mol	Joback Method
hf	-341.44	kJ/mol	Joback Method
hfus	8.20	kJ/mol	Joback Method
hvap	52.06	kJ/mol	Joback Method
log10ws	-1.18		Crippen Method
logp	1.181		Crippen Method

mcvol	87.680	ml/mol	McGowan Method
pc	4769.39	kPa	Joback Method
rinpol	1021.00		NIST Webbook
rinpol	166.55		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1027.00		NIST Webbook
rinpol	166.55		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1021.00		NIST Webbook
ripol	1784.00		NIST Webbook
ripol	1831.00		NIST Webbook
ripol	1832.00		NIST Webbook
ripol	1839.00		NIST Webbook
ripol	1831.00		NIST Webbook
ripol	1827.00		NIST Webbook
ripol	1830.00		NIST Webbook
ripol	1818.00		NIST Webbook
ripol	1831.00		NIST Webbook
ripol	1831.00		NIST Webbook
ripol	1831.00		NIST Webbook
ripol	1829.00		NIST Webbook
ripol	1806.00		NIST Webbook

ripol	1839.00		NIST Webbook
ripol	1800.00		NIST Webbook
ripol	1830.00		NIST Webbook
ripol	1830.00		NIST Webbook
ripol	1799.00		NIST Webbook
ripol	1837.00		NIST Webbook
ripol	1807.00		NIST Webbook
ripol	1831.00		NIST Webbook
ripol	1832.00		NIST Webbook
ripol	1834.00		NIST Webbook
ripol	1829.00		NIST Webbook
ripol	1857.00		NIST Webbook
ripol	1860.00		NIST Webbook
ripol	1816.00		NIST Webbook
ripol	1829.00		NIST Webbook
ripol	1837.00		NIST Webbook
ripol	1861.00		NIST Webbook
ripol	1824.00		NIST Webbook
ripol	1830.00		NIST Webbook
ripol	1833.00		NIST Webbook
ripol	1839.00		NIST Webbook
ripol	1811.00		NIST Webbook
ripol	1830.00		NIST Webbook
tb	525.75	K	Joback Method
tc	734.16	K	Joback Method
tf	327.36	K	Joback Method
vc	0.326	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.77	J/mol×K	525.75	Joback Method
cpg	203.09	J/mol×K	560.48	Joback Method
cpg	212.03	J/mol×K	595.22	Joback Method
cpg	220.57	J/mol×K	629.95	Joback Method
cpg	228.72	J/mol×K	664.69	Joback Method
cpg	236.47	J/mol×K	699.42	Joback Method
cpg	243.81	J/mol×K	734.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80717&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