

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

Other names:	3-Hydroxy-2-methyl-cyclopent-2-enone 3-Hydroxy-2-methyl-2-cyclopenten-1-one
Inchi:	InChI=1S/C6H8O2/c1-4-5(7)2-3-6(4)8/h7H,2-3H2,1H3
InchiKey:	MAIUFLILEAIYBX-UHFFFAOYSA-N
Formula:	C6H8O2
SMILES:	CC1=C(O)CCC1=O
Mol. weight [g/mol]:	112.13
CAS:	5870-63-3

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
ie	8.84 ± 0.05	eV	NIST Webbook
log10ws	-1.18		Crippen Method
logp	1.181		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
pc	4769.39	kPa	Joback Method
rinpol	1025.00		NIST Webbook
rinpol	1025.00		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/molxK	525.75	Joback Method
cpg	203.09	J/molxK	560.48	Joback Method
cpg	212.03	J/molxK	595.22	Joback Method
cpg	220.57	J/molxK	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=C5870633&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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