

2-Cyclopenten-1-one, 2-hydroxy-3,4,4-trimethyl

Other names:	2-Hydroxy-3,4,4-trimethyl-2-cyclopenten-1-one
Inchi:	InChI=1S/C8H12O2/c1-5-7(10)6(9)4-8(5,2)3/h10H,4H2,1-3H3
InchiKey:	LTRJTLUJZFBIEN-UHFFFAOYSA-N
Formula:	C8H12O2
SMILES:	CC1=C(O)C(=O)CC1(C)C
Mol. weight [g/mol]:	140.18

Physical Properties

Property code	Value	Unit	Source
gf	-201.17	kJ/mol	Joback Method
hf	-387.82	kJ/mol	Joback Method
hfus	8.15	kJ/mol	Joback Method
hvap	55.05	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.817		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
rinpol	1088.00		NIST Webbook
ripol	1753.00		NIST Webbook
ripol	1753.00		NIST Webbook
ripol	1753.00		NIST Webbook
tb	567.08	K	Joback Method
tc	776.99	K	Joback Method
tf	369.56	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.31	J/molxK	567.08	Joback Method
cpg	293.74	J/molxK	602.07	Joback Method
cpg	304.63	J/molxK	637.05	Joback Method
cpg	315.05	J/molxK	672.04	Joback Method
cpg	325.08	J/molxK	707.02	Joback Method

cpg	334.79	J/mol×K	742.01	Joback Method
cpg	344.24	J/mol×K	776.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R218376&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

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

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