

4-Hydroxy-3,5,5-trimethylcyclohex-2-enone

Other names:	2-Cyclohexen-1-one, 4-hydroxy-3,5,5-trimethyl
Inchi:	InChI=1S/C9H14O2/c1-6-4-7(10)5-9(2,3)8(6)11/h4,8,11H,5H2,1-3H3
InchiKey:	RLDREDRZMOWDOA-UHFFFAOYSA-N
Formula:	C9H14O2
SMILES:	CC1=CC(=O)CC(C)(C)C1O
Mol. weight [g/mol]:	154.21
CAS:	14203-59-9

Physical Properties

Property code	Value	Unit	Source
gf	-202.93	kJ/mol	Joback Method
hf	-423.49	kJ/mol	Joback Method
hfus	10.11	kJ/mol	Joback Method
hvap	56.48	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
logp	1.293		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
pc	3392.03	kPa	Joback Method
rinpol	1294.00		NIST Webbook
rinpol	1317.70		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1317.70		NIST Webbook
tb	584.58	K	Joback Method
tc	797.08	K	Joback Method
tf	360.55	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.96	J/molxK	584.58	Joback Method
cpg	345.77	J/molxK	620.00	Joback Method
cpg	358.93	J/molxK	655.41	Joback Method
cpg	371.49	J/molxK	690.83	Joback Method

cpg	383.53	J/mol×K	726.25	Joback Method
cpg	395.11	J/mol×K	761.66	Joback Method
cpg	406.30	J/mol×K	797.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14203599&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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