

2-Hydroxy-3,5,5-trimethyl-cyclohex-2-enone

Other names:	2-Hydroxy-3,5,5-trimethyl-2-cyclohexen-1-one 2-Hydroxyisophorone 2-Cyclohexen-1-one, 2-hydroxy-3,5,5-trimethyl-
Inchi:	InChI=1S/C9H14O2/c1-6-4-9(2,3)5-7(10)8(6)11/h11H,4-5H2,1-3H3
InchiKey:	DWGZTTFGUFHAJX-UHFFFAOYSA-N
Formula:	C9H14O2
SMILES:	CC1=C(O)C(=O)CC(C)(C)C1
Mol. weight [g/mol]:	154.21
CAS:	4883-60-7

Physical Properties

Property code	Value	Unit	Source
gf	-204.85	kJ/mol	Joback Method
hf	-414.62	kJ/mol	Joback Method
hfus	8.64	kJ/mol	Joback Method
hvap	57.45	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	2.208		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
rinpol	1149.80		NIST Webbook
rinpol	1194.00		NIST Webbook
ripol	1675.00		NIST Webbook
ripol	1648.00		NIST Webbook
tb	594.23	K	Joback Method
tc	807.77	K	Joback Method
tf	377.31	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.34	J/mol×K	594.23	Joback Method
cpg	342.50	J/mol×K	629.82	Joback Method

cpg	355.06	J/mol×K	665.41	Joback Method
cpg	367.09	J/mol×K	701.00	Joback Method
cpg	378.65	J/mol×K	736.59	Joback Method
cpg	389.81	J/mol×K	772.18	Joback Method
cpg	400.65	J/mol×K	807.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4883607&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

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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