2,6,6-trimethyl-2-hydroxycyclohexanone

Other names: 2-hydroxy-2,6,6-trimethyl-cyclohexanone
2,2,6-trimethyl-2-hydroxycyclohexanone
Inchi: InChI=1S/C9H16O2/c1-8(2)5-4-6-9(3,11)7(8)10/h11H,4-6H2,1-3H3
InchiKey: FWCGLHYHGUHPRY-UHFFFAOYSA-N
Formula: C9H16O2
SMILES: CC1(C)CCCC(C)(O)C1=O
Mol. weight [g/mol]: 156.22

Physical Properties

Property code	Value	Unit	Source
gf	-228.75	kJ/mol	Joback Method
hf	-454.56	kJ/mol	Joback Method
hfus	2.97	kJ/mol	Joback Method
hvap	54.37	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	1.517		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
rinpol	1093.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1093.00		NIST Webbook
ripol	1601.00		NIST Webbook
ripol	1620.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1557.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1588.00		NIST Webbook
ripol	1561.00		NIST Webbook
ripol	1565.00		NIST Webbook
ripol	1561.00		NIST Webbook
tb	580.68	K	Joback Method
tc	798.49	K	Joback Method
tf	371.17	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.81	J/mol×K	580.68	Joback Method
cpg	365.66	J/mol×K	616.98	Joback Method
cpg	379.75	J/mol×K	653.28	Joback Method
cpg	393.24	J/mol×K	689.58	Joback Method
cpg	406.30	J/mol×K	725.88	Joback Method
cpg	419.10	J/mol×K	762.19	Joback Method
cpg	431.79	J/mol×K	798.49	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R149205&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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