2-Hydroxy-3,5,5-trimethylcyclohexanone

Inchi: InChI=1S/C9H16O2/c1-6-4-9(2,3)5-7(10)8(6)11/h6,8,11H,4-5H2,1-3H3
InchiKey: BPRYUSNPHZLEIX-UHFFFAOYSA-N
Formula: C9H16O2
SMILES: CC1CC(C)(C)CC(=O)C1O
Mol. weight [g/mol]: 156.22

Physical Properties

Property code	Value	Unit	Source
gf	-230.97	kJ/mol	Joback Method
hf	-490.14	kJ/mol	Joback Method
hfus	10.34	kJ/mol	Joback Method
hvap	55.21	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	1.373		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
pc	3188.33	kPa	Joback Method
ripol	1656.00		NIST Webbook
ripol	1656.00		NIST Webbook
tb	575.77	K	Joback Method
tc	785.25	K	Joback Method
tf	343.03	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.01	J/mol×K	575.77	Joback Method
cpg	369.63	J/mol×K	610.68	Joback Method
cpg	384.49	J/mol×K	645.60	Joback Method
cpg	398.67	J/mol×K	680.51	Joback Method
cpg	412.22	J/mol×K	715.43	Joback Method
cpg	425.21	J/mol×K	750.34	Joback Method
cpg	437.70	J/mol×K	785.25	Joback Method

Sources

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=R562306&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume