3-Hexanone, 5-hydroxy-5-methyl

Inchi: InChI=1S/C7H14O2/c1-4-6(8)5-7(2,3)9/h9H,4-5H2,1-3H3
InchiKey: NZOHNQRAGPQKMX-UHFFFAOYSA-N
Formula: C7H14O2
SMILES: CCC(=O)CC(C)(C)O
Mol. weight [g/mol]: 130.18

Physical Properties

Property code	Value	Unit	Source
gf	-254.84	kJ/mol	Joback Method
hf	-461.37	kJ/mol	Joback Method
hfus	12.16	kJ/mol	Joback Method
hvap	53.31	kJ/mol	Joback Method
log10ws	-1.41		Crippen Method
logp	1.127		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
rinpol	1016.00		NIST Webbook
rinpol	1016.00		NIST Webbook
tb	502.38	K	Joback Method
tc	682.23	K	Joback Method
tf	281.82	K	Joback Method
vc	0.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.88	J/mol×K	502.38	Joback Method
cpg	279.60	J/mol×K	532.36	Joback Method
cpg	289.76	J/mol×K	562.33	Joback Method
cpg	299.40	J/mol×K	592.31	Joback Method
cpg	308.52	J/mol×K	622.28	Joback Method
cpg	317.16	J/mol×K	652.26	Joback Method
cpg	325.33	J/mol×K	682.23	Joback Method
dvisc	0.0242619	Pa×s	281.82	Joback Method

dvisc	0.0066100	Pa×s	318.58	Joback Method
dvisc	0.0023568	Pa×s	355.34	Joback Method
dvisc	0.0010196	Pa×s	392.10	Joback Method
dvisc	0.0005092	Pa×s	428.86	Joback Method
dvisc	0.0002838	Pa×s	465.62	Joback Method
dvisc	0.0001723	Pa×s	502.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R89431&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume