2-Hexanone, 4-hydroxy-5-methyl-

Other names: 4-hydroxy-5-methyl-2-hexanone
Inchi: InChI=1S/C7H14O2/c1-5(2)7(9)4-6(3)8/h5,7,9H,4H2,1-3H3
InchiKey: BXQODTBLKZARFD-UHFFFAOYSA-N
Formula: C7H14O2
SMILES: CC(=O)CC(O)C(C)C
Mol. weight [g/mol]: 130.18
CAS: 38836-21-4

Physical Properties

Property code	Value	Unit	Source
gf	-262.56	kJ/mol	Joback Method
hf	-463.18	kJ/mol	Joback Method
hfus	12.53	kJ/mol	Joback Method
hvap	53.83	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	0.982		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3384.14	kPa	Joback Method
rinpol	954.00		NIST Webbook
rinpol	954.00		NIST Webbook
tb	504.73	K	Joback Method
tc	681.69	K	Joback Method
tf	249.40	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.07	J/mol×K	504.73	Joback Method
cpg	276.55	J/mol×K	534.22	Joback Method
cpg	286.57	J/mol×K	563.72	Joback Method
cpg	296.15	J/mol×K	593.21	Joback Method
cpg	305.30	J/mol×K	622.70	Joback Method
cpg	314.03	J/mol×K	652.20	Joback Method

cpg	322.35	J/mol×K	681.69	Joback Method
dvisc	0.0707125	Pa×s	249.40	Joback Method
dvisc	0.0121690	Pa×s	291.95	Joback Method
dvisc	0.0032769	Pa×s	334.51	Joback Method
dvisc	0.0011865	Pa×s	377.06	Joback Method
dvisc	0.0005279	Pa×s	419.62	Joback Method
dvisc	0.0002727	Pa×s	462.18	Joback Method
dvisc	0.0001574	Pa×s	504.73	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=C38836214&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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