2-Hydroxy-5-methyl-3-hexanone

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

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
ripol	1458.00		NIST Webbook
ripol	1456.00		NIST Webbook
ripol	1449.00		NIST Webbook
ripol	1458.00		NIST Webbook
ripol	1456.00		NIST Webbook
ripol	1458.00		NIST Webbook
ripol	1449.00		NIST Webbook
ripol	1453.00		NIST Webbook
ripol	1453.00		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	314.03	J/mol×K	652.20	Joback Method
cpg	305.30	J/mol×K	622.70	Joback Method
cpg	296.15	J/mol×K	593.21	Joback Method
cpg	286.57	J/mol×K	563.72	Joback Method
cpg	276.55	J/mol×K	534.22	Joback Method
cpg	322.35	J/mol×K	681.69	Joback Method
dvisc	0.0001574	Pa×s	504.73	Joback Method
dvisc	0.0002727	Pa×s	462.18	Joback Method
dvisc	0.0005279	Pa×s	419.62	Joback Method
dvisc	0.0011865	Pa×s	377.06	Joback Method
dvisc	0.0032769	Pa×s	334.51	Joback Method
dvisc	0.0121690	Pa×s	291.95	Joback Method
dvisc	0.0707125	Pa×s	249.40	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R516695&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume