4-Octanone, 5-hydroxy-2,7-dimethyl-

Other names: 5-Hydroxy 2,7-dimethyl 4-octanone
Inchi: InChI=1S/C10H20O2/c1-7(2)5-9(11)10(12)6-8(3)4/h7-9,11H,5-6H2,1-4H3
InchiKey: NVLCZXVVPKJWST-UHFFFAOYSA-N
Formula: C10H20O2
SMILES: CC(C)CC(=O)C(O)CC(C)C
Mol. weight [g/mol]: 172.26
CAS: 6838-51-3

Physical Properties

Property code	Value	Unit	Source
gf	-239.74	kJ/mol	Joback Method
hf	-530.38	kJ/mol	Joback Method
hfus	16.77	kJ/mol	Joback Method
hvap	60.11	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	2.009		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
tb	572.93	K	Joback Method
tc	748.66	K	Joback Method
tf	268.21	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.87	J/mol×K	572.93	Joback Method
cpg	417.12	J/mol×K	602.22	Joback Method
cpg	429.76	J/mol×K	631.51	Joback Method
cpg	441.83	J/mol×K	660.79	Joback Method
cpg	453.33	J/mol×K	690.08	Joback Method
cpg	464.28	J/mol×K	719.37	Joback Method
cpg	474.69	J/mol×K	748.66	Joback Method
dvisc	0.0637662	Pa×s	268.21	Joback Method

dvisc	0.0088269	Pa×s	319.00	Joback Method
dvisc	0.0021034	Pa×s	369.78	Joback Method
dvisc	0.0007087	Pa×s	420.57	Joback Method
dvisc	0.0003019	Pa×s	471.36	Joback Method
dvisc	0.0001518	Pa×s	522.14	Joback Method
dvisc	0.0000862	Pa×s	572.93	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6838513&Units=SI

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

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