2-Pentanone, 4-hydroxy-

Other names: CH3CH(OH)CH2C(O)CH3
4-Hydroxy-4-methyl-2-butanone
4-hydroxypentan-2-one
Inchi: InChI=1S/C5H10O2/c1-4(6)3-5(2)7/h4,6H,3H2,1-2H3
InchiKey: PCYZZYAEGNVNMH-UHFFFAOYSA-N
Formula: C5H10O2
SMILES: CC(=O)CC(C)O
Mol. weight [g/mol]: 102.13
CAS: 4161-60-8

Physical Properties

Property code	Value	Unit	Source
gf	-276.96	kJ/mol	Joback Method
hf	-416.62	kJ/mol	Joback Method
hfus	10.87	kJ/mol	Joback Method
hvap	49.76	kJ/mol	Joback Method
log10ws	-0.57		Crippen Method
logp	0.346		Crippen Method
mcvol	88.750	ml/mol	McGowan Method
pc	4244.08	kPa	Joback Method
rinpol	822.00		NIST Webbook
rinpol	849.40		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	818.00		NIST Webbook
tb	450.15 ± 3.00	K	NIST Webbook
tb	450.15 ± 2.00	K	NIST Webbook
tc	635.76	K	Joback Method
tf	241.86	K	Joback Method
vc	0.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.94	J/mol×K	459.41	Joback Method

cpg	220.97	J/mol×K	606.37	Joback Method
cpg	214.20	J/mol×K	576.97	Joback Method
cpg	207.12	J/mol×K	547.58	Joback Method
cpg	199.72	J/mol×K	518.19	Joback Method
cpg	191.99	J/mol×K	488.80	Joback Method
cpg	227.44	J/mol×K	635.76	Joback Method
dvisc	0.0002315	Pa×s	459.41	Joback Method
dvisc	0.0003892	Pa×s	423.15	Joback Method
dvisc	0.0007211	Pa×s	386.89	Joback Method
dvisc	0.0015179	Pa×s	350.63	Joback Method
dvisc	0.0037936	Pa×s	314.38	Joback Method
dvisc	0.0120393	Pa×s	278.12	Joback Method
dvisc	0.0540168	Pa×s	241.86	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4161608&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