1-Hydroxy-2-pentanone

Other names: 2-Pentanone, 1-hydroxy-
Inchi: InChI=1S/C5H10O2/c1-2-3-5(7)4-6/h6H,2-4H2,1H3
InchiKey: WOVLKKLXYZJMSN-UHFFFAOYSA-N
Formula: C5H10O2
SMILES: CCCC(=O)CO
Mol. weight [g/mol]: 102.13
CAS: 64502-89-2

Physical Properties

Property code	Value	Unit	Source
gf	-274.52	kJ/mol	Joback Method
hf	-411.34	kJ/mol	Joback Method
hfus	14.39	kJ/mol	Joback Method
hvap	50.15	kJ/mol	Joback Method
log10ws	-0.46		Crippen Method
logp	0.348		Crippen Method
mcvol	88.750	ml/mol	McGowan Method
pc	4200.18	kPa	Joback Method
rinpol	695.00		NIST Webbook
rinpol	695.00		NIST Webbook
ripol	1469.00		NIST Webbook
ripol	1445.00		NIST Webbook
ripol	1439.00		NIST Webbook
ripol	1469.00		NIST Webbook
tb	459.85	K	Joback Method
tc	632.49	K	Joback Method
tf	256.86	K	Joback Method
vc	0.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.75	J/mol×K	459.85	Joback Method
cpg	191.56	J/mol×K	488.62	Joback Method

cpg	199.06	J/mol×K	517.40	Joback Method
cpg	206.25	J/mol×K	546.17	Joback Method
cpg	213.15	J/mol×K	574.94	Joback Method
cpg	219.76	J/mol×K	603.72	Joback Method
cpg	226.08	J/mol×K	632.49	Joback Method
dvisc	0.0272118	Pa×s	256.86	Joback Method
dvisc	0.0078379	Pa×s	290.69	Joback Method
dvisc	0.0029265	Pa×s	324.52	Joback Method
dvisc	0.0013161	Pa×s	358.36	Joback Method
dvisc	0.0006794	Pa×s	392.19	Joback Method
dvisc	0.0003895	Pa×s	426.02	Joback Method
dvisc	0.0002424	Pa×s	459.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64502892&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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