2-Hydroxy-3-pentanone

Other names: 3-Pentanone, 2-hydroxy-
3-Pentanon-2-ol
Inchi: InChI=1S/C5H10O2/c1-3-5(7)4(2)6/h4,6H,3H2,1-2H3
InchiKey: QMXCHEVUAIPIRM-UHFFFAOYSA-N
Formula: C5H10O2
SMILES: CCC(=O)C(C)O
Mol. weight [g/mol]: 102.13
CAS: 5704-20-1

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	821.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	777.00		NIST Webbook
ripol	1368.00		NIST Webbook
ripol	1351.00		NIST Webbook
ripol	1380.00		NIST Webbook
ripol	1370.00		NIST Webbook
ripol	1366.00		NIST Webbook
ripol	1364.00		NIST Webbook
ripol	1361.00		NIST Webbook
ripol	1351.00		NIST Webbook
ripol	1366.00		NIST Webbook
ripol	1386.00		NIST Webbook
ripol	1351.00		NIST Webbook
ripol	1386.00		NIST Webbook

ripol	1396.00		NIST Webbook
ripol	1355.00		NIST Webbook
ripol	1361.00		NIST Webbook
tb	459.41	K	Joback Method
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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5704201&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

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