2-Pentanone, 5-(acetyloxy)-

Other names:	2-Pentanone, 5-hydroxy-, acetate
	«gamma»-Acetylpropyl acetate
	Acetopropyl acetate
	3-Acetylpropyl acetate
	4-Ketovaleryl acetate
	4-Oxopentyl acetate
	5-Acetoxypentan-2-one
	CH3C(O)O(CH2)3C(O)CH3
	5-Hydroxy-2-pentanone acetate
	1-Acetoxy-4-pentanone
Inchi:	InChI=1S/C7H12O3/c1-6(8)4-3-5-10-7(2)9/h3-5H2,1-2H3
InchiKey:	QYAHGDMPUORRQD-UHFFFAOYSA-N
Formula:	C7H12O3
SMILES:	CC(=O)CCCOC(C)=O
Mol. weight [g/mol]:	144.17
CAS:	5185-97-7

Physical Properties

Property code	Value	Unit	Source
gf	-354.78	kJ/mol	Joback Method
hf	-545.19	kJ/mol	Joback Method
hfus	18.27	kJ/mol	Joback Method
hvap	47.08	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	0.919		Crippen Method
mcvol	118.500	ml/mol	McGowan Method
pc	3152.62	kPa	Joback Method
rinpol	1053.00		NIST Webbook
tb	489.72	K	Joback Method
tc	676.50	K	Joback Method
tf	290.74	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.79	J/mol×K	489.72	Joback Method
cpg	266.32	J/mol×K	520.85	Joback Method
cpg	276.45	J/mol×K	551.98	Joback Method
cpg	286.16	J/mol×K	583.11	Joback Method
cpg	295.47	J/mol×K	614.24	Joback Method
cpg	304.37	J/mol×K	645.37	Joback Method
cpg	312.87	J/mol×K	676.50	Joback Method
dvisc	0.0027292	Pa×s	290.74	Joback Method
dvisc	0.0015623	Pa×s	323.90	Joback Method
dvisc	0.0009920	Pa×s	357.07	Joback Method
dvisc	0.0006804	Pa×s	390.23	Joback Method
dvisc	0.0004951	Pa×s	423.39	Joback Method
dvisc	0.0003773	Pa×s	456.56	Joback Method
dvisc	0.0002983	Pa×s	489.72	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=C5185977&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume