2-Propanone, 1-(acetyloxy)-

Other names:	2-Propanone, 1-hydroxy-, acetate
	Acetol acetate
	Acetonyl acetate
	Acetoxyacetone
	Acetoxypropanone
	Acetylmethyl acetate
	O-Acetylacetol
	1-Acetoxy-2-propanone
	1-Acetoxyacetone
	1-Hydroxy-2-propanone acetate
	2-Oxopropyl acetate
	1-(Acetyloxy)-2-propanone
	1-Acetoxy-propan-2-one
	1-Acetyloxy-propan-2-one
	Acetoxy-2-propanone
	NSC 2298
	NSC 7614
	Hydroxyacetone, acetate
Inchi:	InChI=1S/C5H8O3/c1-4(6)3-8-5(2)7/h3H2,1-2H3
InchiKey:	DBERHVIZRVGDFO-UHFFFAOYSA-N
Formula:	C5H8O3
SMILES:	CC(=O)COC(C)=O
Mol. weight [g/mol]:	116.12
CAS:	592-20-1

Physical Properties

Property code	Value	Unit	Source
gf	-371.62	kJ/mol	Joback Method
hf	-503.91	kJ/mol	Joback Method
hfus	13.09	kJ/mol	Joback Method
hvap	42.63	kJ/mol	Joback Method
log10ws	-0.06		Crippen Method
logp	0.138		Crippen Method
mcvol	90.320	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
rinpol	839.00		NIST Webbook
rinpol	870.00		NIST Webbook

rinpol	826.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	869.00		NIST Webbook
ripol	1483.00		NIST Webbook
ripol	1484.00		NIST Webbook
ripol	1478.00		NIST Webbook
ripol	1467.00		NIST Webbook
ripol	1483.00		NIST Webbook
ripol	1470.00		NIST Webbook
ripol	1454.00		NIST Webbook
ripol	1465.00		NIST Webbook
ripol	1478.00		NIST Webbook
ripol	1484.00		NIST Webbook
ripol	1484.00		NIST Webbook
ripol	1469.00		NIST Webbook
ripol	1477.00		NIST Webbook
ripol	1477.00		NIST Webbook
tb	447.00	K	NIST Webbook
tc	634.74	K	Joback Method
tf	268.20	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.41	J/mol×K	443.96	Joback Method
cpg	184.43	J/mol×K	475.76	Joback Method
cpg	192.17	J/mol×K	507.55	Joback Method
cpg	199.65	J/mol×K	539.35	Joback Method
cpg	206.83	J/mol×K	571.15	Joback Method

cpg	213.74	J/mol×K	602.95	Joback Method
cpg	220.34	J/mol×K	634.74	Joback Method
dvisc	0.0025634	Pa×s	268.20	Joback Method
dvisc	0.0015356	Pa×s	297.49	Joback Method
dvisc	0.0010084	Pa×s	326.79	Joback Method
dvisc	0.0007096	Pa×s	356.08	Joback Method
dvisc	0.0005268	Pa×s	385.37	Joback Method
dvisc	0.0004079	Pa×s	414.67	Joback Method
dvisc	0.0003266	Pa×s	443.96	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	347.00	K	2.40	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C592201&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume