2-Butanone, 1-(acetyloxy)-

Other names:	2-Butanone, 1-hydroxy-, acetate
	1-Acetoxy-2-butanone
	1-Hydroxy-2-butanone acetate
	2-Oxobutyl acetate
	1-Acetoxy-butan-2-one
	1-(Acetyloxy)-2-butanone
Inchi:	InChI=1S/C6H10O3/c1-3-6(8)4-9-5(2)7/h3-4H2,1-2H3
InchiKey:	LHGWJCBYBIICPP-UHFFFAOYSA-N
Formula:	C6H10O3
SMILES:	CCC(=O)COC(C)=O
Mol. weight [g/mol]:	130.14
CAS:	1575-57-1

Physical Properties

Property code	Value	Unit	Source
gf	-363.20	kJ/mol	Joback Method
hf	-524.55	kJ/mol	Joback Method
hfus	15.68	kJ/mol	Joback Method
hvap	44.85	kJ/mol	Joback Method
log10ws	-0.48		Crippen Method
logp	0.529		Crippen Method
mcvol	104.410	ml/mol	McGowan Method
pc	3522.09	kPa	Joback Method
rinpol	985.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	985.00		NIST Webbook
ripol	1553.00		NIST Webbook
ripol	1554.00		NIST Webbook
ripol	1553.00		NIST Webbook
ripol	1526.00		NIST Webbook
ripol	1553.00		NIST Webbook
ripol	1521.00		NIST Webbook
ripol	1536.00		NIST Webbook
ripol	1556.00		NIST Webbook

ripol	1554.00		NIST Webbook
ripol	1554.00		NIST Webbook
ripol	1526.00		NIST Webbook
ripol	1521.00		NIST Webbook
ripol	1536.00		NIST Webbook
ripol	1554.00		NIST Webbook
ripol	1526.00		NIST Webbook
tb	466.84	K	Joback Method
tc	655.65	K	Joback Method
tf	279.47	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.00	J/mol×K	466.84	Joback Method
cpg	224.34	J/mol×K	498.31	Joback Method
cpg	233.35	J/mol×K	529.78	Joback Method
cpg	242.00	J/mol×K	561.25	Joback Method
cpg	250.31	J/mol×K	592.71	Joback Method
cpg	258.27	J/mol×K	624.18	Joback Method
cpg	265.88	J/mol×K	655.65	Joback Method
dvisc	0.0026736	Pa×s	279.47	Joback Method
dvisc	0.0015646	Pa×s	310.70	Joback Method
dvisc	0.0010097	Pa×s	341.93	Joback Method
dvisc	0.0007012	Pa×s	373.16	Joback Method
dvisc	0.0005151	Pa×s	404.38	Joback Method
dvisc	0.0003956	Pa×s	435.61	Joback Method
dvisc	0.0003147	Pa×s	466.84	Joback Method

Sources

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=C1575571&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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