Acetic acid, (acetyloxy)-

Other names:	Glycolic acid, acetate
	(Acetyloxy)acetic acid
	«alpha»-Acetoxyacetic acid
	2-Hydroxyacetic acid acetata
	Acetoxyacetic acid
	Acetylglycolic acid
	O-Acetylglycolic acid
	Acetic acid, 2-(acetyloxy)-
Inchi:	InChI=1S/C4H6O4/c1-3(5)8-2-4(6)7/h2H2,1H3,(H,6,7)
InchiKey:	MLXDUYUQINCFFV-UHFFFAOYSA-N
Formula:	C4H6O4
SMILES:	CC(=O)OCC(=O)O
Mol. weight [g/mol]:	118.09
CAS:	13831-30-6

Physical Properties

Property code	Value	Unit	Source
gf	-516.86	kJ/mol	Joback Method
hf	-635.50	kJ/mol	Joback Method
hfus	14.59	kJ/mol	Joback Method
hvap	57.08	kJ/mol	Joback Method
log10ws	0.54		Crippen Method
logp	-0.366		Crippen Method
mcvol	82.100	ml/mol	McGowan Method
pc	5094.76	kPa	Joback Method
rinpol	1019.80		NIST Webbook
tb	513.26	K	Joback Method
tc	696.47	K	Joback Method
tf	340.00 ± 1.00	K	NIST Webbook
vc	0.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	174.45	J/mol×K	513.26	Joback Method
cpg	180.44	J/mol×K	543.80	Joback Method
cpg	186.21	J/mol×K	574.33	Joback Method
cpg	191.75	J/mol×K	604.87	Joback Method
cpg	197.06	J/mol×K	635.40	Joback Method
cpg	202.13	J/mol×K	665.94	Joback Method
cpg	206.96	J/mol×K	696.47	Joback Method
dvisc	0.0068490	Pa×s	317.75	Joback Method
dvisc	0.0028285	Pa×s	350.33	Joback Method
dvisc	0.0013579	Pa×s	382.92	Joback Method
dvisc	0.0007314	Pa×s	415.50	Joback Method
dvisc	0.0004310	Pa×s	448.09	Joback Method
dvisc	0.0002729	Pa×s	480.68	Joback Method
dvisc	0.0001831	Pa×s	513.26	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	414.70	K	1.60	NIST Webbook
tbrp	417.70	K	1.60	NIST Webbook
tbrp	418.00	K	1.60	NIST Webbook

Sources

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=C13831306&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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