2-ACETOXY-1-PROPANOL

Other names: Acetic acid, 2-hydroxy-1-methylethyl ester
2-Acetoxy-1-propanol
Inchi: InChI=1S/C5H10O3/c1-4(3-6)8-5(2)7/h4,6H,3H2,1-2H3
InchiKey: YJNKLTDJZSXVHQ-UHFFFAOYSA-N
Formula: C5H10O3
SMILES: CC(=O)OC(C)CO
Mol. weight [g/mol]: 118.13

Physical Properties

Property code	Value	Unit	Source
af	0.6229		Cheméo Relay (1.0)
hf	-664.10	kJ/mol	Cheméo Relay (1.0)
hfus	12.06	kJ/mol	Joback Method
hvap	64.26	kJ/mol	Cheméo Relay (1.0)
ie	10.23	eV	Cheméo Relay (1.0)
log10ws	0.35		Cheméo Relay (1.0)
logp	-0.070		Crippen Method
mcvol	94.620	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
rinpol	891.10		NIST Webbook
rinpol	891.10		NIST Webbook
ripol	1617.00		NIST Webbook
ripol	1621.00		NIST Webbook
ripol	1617.00		NIST Webbook
ripol	1621.00		NIST Webbook
tb	436.49	K	Cheméo Relay (1.0)
tc	616.49	K	Cheméo Relay (1.0)
tf	237.76	K	Cheméo Relay (1.0)
vc	0.350	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.80	J/mol×K	481.83	Joback Method

cpg	212.77	J/mol×K	511.13	Joback Method
cpg	220.46	J/mol×K	540.44	Joback Method
cpg	227.87	J/mol×K	569.74	Joback Method
cpg	235.00	J/mol×K	599.05	Joback Method
cpg	241.86	J/mol×K	628.35	Joback Method
cpg	248.43	J/mol×K	657.66	Joback Method
dvisc	0.0255824	Pa×s	264.09	Joback Method
dvisc	0.0067671	Pa×s	300.38	Joback Method
dvisc	0.0023843	Pa×s	336.67	Joback Method
dvisc	0.0010292	Pa×s	372.96	Joback Method
dvisc	0.0005156	Pa×s	409.25	Joback Method
dvisc	0.0002891	Pa×s	445.54	Joback Method
dvisc	0.0001769	Pa×s	481.83	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6214013&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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

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

Cheméo Relay (1.0):

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

ie: Ionization energy

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