

Propanoic acid, 2-hydroxy-2-methyl-, ethyl ester

Other names:	Lactic acid, 2-methyl-, ethyl ester Ethyl «alpha»-hydroxyisobutyrate Ethyl 2-hydroxy-2-methylpropionate Ethyl 2-hydroxyisobutyrate Ethyl 2-methylactate 2-Methylactic acid ethyl ester
Inchi:	InChI=1S/C6H12O3/c1-4-9-5(7)6(2,3)8/h8H,4H2,1-3H3
InchiKey:	GFUIDHWFLMPAGY-UHFFFAOYSA-N
Formula:	C6H12O3
SMILES:	CCOC(=O)C(C)(C)O
Mol. weight [g/mol]:	132.16
CAS:	80-55-7

Physical Properties

Property code	Value	Unit	Source
gf	-368.26	kJ/mol	Joback Method
hf	-572.95	kJ/mol	Joback Method
hfus	10.76	kJ/mol	Joback Method
hvap	53.49	kJ/mol	Joback Method
log10ws	-0.57		Crippen Method
logp	0.320		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3731.66	kPa	Joback Method
tb	423.20	K	NIST Webbook
tc	682.72	K	Joback Method
tf	292.78	K	Joback Method
vc	0.404	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.95	J/mol×K	501.92	Joback Method
cpg	292.32	J/mol×K	652.58	Joback Method
cpg	284.51	J/mol×K	622.45	Joback Method

cpg	276.27	J/molxK	592.32	Joback Method
cpg	267.61	J/molxK	562.19	Joback Method
cpg	258.51	J/molxK	532.05	Joback Method
cpg	299.73	J/molxK	682.72	Joback Method
dvisc	0.0001543	Paxs	501.92	Joback Method
dvisc	0.0002484	Paxs	467.06	Joback Method
dvisc	0.0004319	Paxs	432.21	Joback Method
dvisc	0.0008275	Paxs	397.35	Joback Method
dvisc	0.0017968	Paxs	362.49	Joback Method
dvisc	0.0046012	Paxs	327.64	Joback Method
dvisc	0.0147388	Paxs	292.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80557&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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