Propanoic acid, 2-hydroxy-2-methyl-

Other names:	(CH3)2COHCOOH
	2-Hydroxy-2-methylpropionic acid
	2-hydroxy-2-methylpropanoic acid
	2-hydroxyisobutyric acid
	2-methyllactic acid
	Acetonic acid
	Hydroxydimethylacetic acid
	Lactic acid, 2-methyl-
	NSC 402158
	NSC 4505
	Propanoic acid, 2-methyl-2-hydroxy-
	«alpha»-Hydroxyisobutanoic acid
	«alpha»-Hydroxyisobutyric acid
Inchi:	InChI=1S/C4H8O3/c1-4(2,7)3(5)6/h7H,1-2H3,(H,5,6)
InchiKey:	BWLBGMIXKSTLSX-UHFFFAOYSA-N
Formula:	C4H8O3
SMILES:	CC(C)(O)C(=O)O
Mol. weight [g/mol]:	104.10
CAS:	594-61-6

Physical Properties

Property code	Value	Unit	Source
gf	-416.92	kJ/mol	Joback Method
hf	-551.68	kJ/mol	Joback Method
hfus	8.48	kJ/mol	Joback Method
hvap	63.31	kJ/mol	Joback Method
ie	10.90 ± 0.10	eV	NIST Webbook
log10ws	0.03		Crippen Method
logp	-0.158		Crippen Method
mcvol	80.530	ml/mol	McGowan Method
pc	5602.57	kPa	Joback Method
ripol	1918.00		NIST Webbook
ripol	1918.00		NIST Webbook
tb	485.20	K	NIST Webbook
tc	702.65	K	Joback Method
tf	354.00 ± 3.00	K	NIST Webbook
vc	0.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.87	J/mol×K	702.65	Joback Method
cpg	186.31	J/mol×K	525.92	Joback Method
cpg	192.59	J/mol×K	555.38	Joback Method
cpg	198.50	J/mol×K	584.83	Joback Method
cpg	204.06	J/mol×K	614.29	Joback Method
cpg	209.30	J/mol×K	643.74	Joback Method
cpg	214.23	J/mol×K	673.20	Joback Method
dvisc	0.0000844	Pa×s	525.92	Joback Method
dvisc	0.0401709	Pa×s	308.83	Joback Method
dvisc	0.0083870	Pa×s	345.01	Joback Method
dvisc	0.0023575	Pa×s	381.19	Joback Method
dvisc	0.0008258	Pa×s	417.38	Joback Method
dvisc	0.0003419	Pa×s	453.56	Joback Method
dvisc	0.0001613	Pa×s	489.74	Joback Method
hvapt	67.50	kJ/mol	428.00	NIST Webbook
rhos	1240.00	kg/m3	293.00	Thermodynamic properties of 2-methyl lactic acid

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	357.20	K	0.10	NIST Webbook

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=C594616&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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rhos:	Solid Density
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