Malic Acid

Other names:	(.+/-.)-Malic acid
	2-Hydroxyethane-1,2-dicarboxylic acid
	Butanedioic acid, 2-hydroxy-
	Butanedioic acid, hydroxy-
	DEOXYTETRARIC ACID
	FDA 2018
	HYDROXYBUTANEDIOIC ACID
	Hydroxyethane-1,2-dicarboxylic acid
	Hydroxysuccinic acid
	Kyselina hydroxybutandiova
	Kyselina jablecna
	Musashi-no-Ringosan
	NSC 25941
	POMALUS ACID
	R,S(.+/-.)-Malic acid
	Succinic acid, hydroxy-
	dl-Malic acid
	«alpha»-Hydroxysuccinic acid
	Â«alphaÂ»-Hydroxysuccinic acid
Inchi:	InChI=1S/C4H6O5/c5-2(4(8)9)1-3(6)7/h2,5H,1H2,(H,6,7)(H,8,9)
InchiKey:	BJEPYKJPYRNKOW-UHFFFAOYSA-N
Formula:	C4H6O5
SMILES:	O=C(O)CC(O)C(=O)O
Mol. weight [g/mol]:	134.09
CAS:	6915-15-7

Physical Properties

Property code	Value	Unit	Source
gf	-687.94	kJ/mol	Joback Method
hf	-813.02	kJ/mol	Joback Method
hfus	18.05	kJ/mol	Joback Method
hvap	87.64	kJ/mol	Joback Method
log10ws	0.93		Crippen Method
logp	-1.093		Crippen Method
mcvol	87.970	ml/mol	McGowan Method
pc	7037.97	kPa	Joback Method
tb	674.76	K	Joback Method

tc	849.14	K	Joback Method
tf	403.15	K	Thermodynamic models for determination of the solubility of DL-malic acid in methanol plus (acetonitrile, N,N-dimethylformamide, isopropyl alcohol) binary solvent mixtures
tf	400.75 ± 0.60	K	NIST Webbook
vc	0.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.47	J/mol×K	674.76	Joback Method
cpg	227.04	J/mol×K	703.82	Joback Method
cpg	231.36	J/mol×K	732.89	Joback Method
cpg	235.42	J/mol×K	761.95	Joback Method
cpg	239.25	J/mol×K	791.02	Joback Method
cpg	242.84	J/mol×K	820.08	Joback Method
cpg	246.21	J/mol×K	849.14	Joback Method
dvisc	0.0048344	Pa×s	402.16	Joback Method
dvisc	0.0009670	Pa×s	447.59	Joback Method
dvisc	0.0002602	Pa×s	493.03	Joback Method
dvisc	0.0000874	Pa×s	538.46	Joback Method
dvisc	0.0000348	Pa×s	583.89	Joback Method
dvisc	0.0000158	Pa×s	629.33	Joback Method
dvisc	0.0000080	Pa×s	674.76	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.51357e+02
Coeff. B	-2.63327e+04
Coeff. C	-3.22403e+01
Coeff. D	9.21419e-06
Temperature range (K), min.	403.15

Temperature range (K), max.	781.00

Sources

Surface Tensions and Densities of Oxalic, Malonic, Succinic, Maleic, Malic, and cis-Pinonic Acids:	https://www.doi.org/10.1021/je050366x
Effects of Different Organic Acids on Solubility and Metastable Zone Width of Zinc Lactate:	https://www.doi.org/10.1021/je3006453
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Low transition temperature mixtures (LTTMs) as novel entrainers in extractive distillation:	https://www.doi.org/10.1016/j.fluid.2014.10.044
Thermodynamic models for determination of the solubility of DL-malic acid in methanol plus acetonitrile, N,N-dimethylformamide, isopropyl alcohol) binary solvent mixtures:	https://www.doi.org/10.1016/j.jct.2015.02.002
Synthesis and Physical and Thermodynamic Properties of Lactic Acid Vapor Pressure Data:	https://www.doi.org/10.1021/acs.jced.7b01037
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=977
Deep Eutectic Solvents:	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6915157&Units=SI
Experiment and correlation of osmotic coefficient for aqueous solution of carboxylic acids using NRTL nonrandom factor model:	https://www.doi.org/10.1016/j.fluid.2012.05.002
Surface Tension of Aqueous Solutions of Small Chain Amino and Organic Acids:	https://www.doi.org/10.1021/acs.jced.9b00026
Solubility of DL-malic acid in water, ethanol and in mixtures of ethanol + water :	https://www.doi.org/10.1016/j.fluid.2014.06.017
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=977
Solubility of citric, malonic, and malic acids in different solvents from 303.2 to 333.2 K:	https://www.doi.org/10.1016/j.fluid.2011.09.033

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

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