Citric acid

Other names:	1,2,3-Propanetricarboxylic acid, 2-hydroxy-
	2-Hydroxy-1,2,3-propanetricarboxylic acid
	3-Carboxy-3-hydroxypentane-1,5-dioic acid
	Aciletten
	Anhydrous citric acid
	Chemfill
	Citretten
	Citric acid, anhydrous
	Citro
	F 0001 (polycarboxylic acid)
	Hydrocerol A
	Kyselina 2-hydroxy-1,2,3-propantrikarbonova
	Kyselina citronova
	NSC 30279
	NSC 626579
	«beta»-Hydroxytricarballylic acid
	Â«betaÂ»-Hydroxytricarballylic acid
Inchi:	InChI=1S/C6H8O7/c7-3(8)1-6(13,5(11)12)2-4(9)10/h13H,1-2H2,(H,7,8)(H,9,10)(H,11,12)
InchiKey:	KRKNYBCHXYNGOX-UHFFFAOYSA-N
Formula:	C6H8O7
SMILES:	O=C(O)CC(O)(CC(=O)O)C(=O)O
Mol. weight [g/mol]:	192.12
CAS:	77-92-9

Physical Properties

Property code	Value	Unit	Source
chs	-1960.60 ± 4.60	kJ/mol	NIST Webbook
gf	-931.56	kJ/mol	Joback Method
hf	-1122.58	kJ/mol	Joback Method
hfs	-1543.80 ± 4.60	kJ/mol	NIST Webbook
hfus	25.03	kJ/mol	Joback Method
hvap	114.61	kJ/mol	Joback Method
log10ws	0.51		Aqueous Solubility Prediction Method
logp	-1.249		Crippen Method
mcvol	123.590	ml/mol	McGowan Method
pc	6740.71	kPa	Joback Method

ss	252.10	J/mol×K	NIST Webbook
tb	863.78	K	Joback Method
tc	1058.50	K	Joback Method
tf	427.15 ± 1.50	K	NIST Webbook
tf	428.55	K	DSC study and phase diagrams calculation of binary systems of paracetamol
tf	426.40	K	Aqueous Solubility Prediction Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.51	J/mol×K	863.78	Joback Method
cpg	359.94	J/mol×K	896.23	Joback Method
cpg	364.04	J/mol×K	928.69	Joback Method
cpg	367.86	J/mol×K	961.14	Joback Method
cpg	371.41	J/mol×K	993.59	Joback Method
cpg	374.73	J/mol×K	1026.04	Joback Method
cpg	377.85	J/mol×K	1058.50	Joback Method
cps	226.51	J/mol×K	300.00	NIST Webbook
dvisc	0.0000736	Pa×s	552.87	Joback Method
dvisc	0.0000190	Pa×s	604.69	Joback Method
dvisc	0.0000061	Pa×s	656.51	Joback Method
dvisc	0.0000023	Pa×s	708.33	Joback Method
dvisc	0.0000010	Pa×s	760.14	Joback Method
dvisc	0.0000005	Pa×s	811.96	Joback Method
dvisc	0.0000002	Pa×s	863.78	Joback Method

Sources

Solubility of citric acid in water, ethanol, n-propanol and in mixtures of ethanol + water.	https://www.doi.org/10.1016/j.fluid.2013.05.014
Thermodynamic properties of aqueous solutions with citrate ions.	https://www.doi.org/10.1016/j.jct.2013.04.017
McGowan Method: Compressibility studies in aqueous solutions of citric acid:	http://link.springer.com/article/10.1007/BF02311772
Solubility modelling and thermodynamic properties of allopurinol in aqueous solutions of four deep eutectic solvents.	https://www.doi.org/10.1016/j.jct.2019.01.018
Effect of Hydrogen Bond Donor on the Physical Properties of Benzyltrimethylammonium Chloride Based Deep Eutectic Solvents and Their Usage in 2-Ethyl-Hexyl Acetate Synthesis as a Catalyst.	https://www.doi.org/10.1021/acs.jced.6b00486
Densities and Viscosities of Citric Acid in Aqueous Cetrimonium Bromide	https://www.doi.org/10.1021/je2000217
Physical properties of seven deep eutectic solvents based on L-proline or betaine:	https://www.doi.org/10.1016/j.jct.2018.12.017

Solubilities of 3-Carboxy-3-hydroxypentanedioic Acid in Ethanol, Butan-1-ol, Water, Acetone, and Methylbenzene:	https://www.doi.org/10.1021/je101167z
Coupled diffusion in aqueous citric acid + calcium citrate solutions:	https://www.doi.org/10.1016/j.jct.2018.11.003
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
DSC study and phase diagrams calculation of binary systems of paracetamol:	https://www.doi.org/10.1016/j.tca.2012.09.024
Influence of Imidazolium Ionic Liquids on the Interactions of Human Hemoglobin with DyCl3, ErCl3, and YbCl3 in Aqueous Citric Acid at T = (298.15, 303.15, and 308.15) K and 0.1 MPa:	https://www.doi.org/10.1021/acs.jced.6b00695
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
Solubilities of Three Flavonoids in Different Natural Deep Eutectic Solvents at T = (288.15 to 328.15) K:	https://www.doi.org/10.1021/acs.jced.6b00552
Solubility and Mass Transfer Coefficient Enhancement of Benzyl Acetate in Water through Hydrotropy:	https://www.doi.org/10.1021/je0342872
Molar Heat Capacity of Selected Type III Deep Eutectic Solvents :	https://www.doi.org/10.1021/acs.jced.5b00989
Solubility of 2-Hydroxypropane-1,2,3-tricarboxylic Acid Monohydrate in Different Binary Solvents from (278.15 to 303.15) K:	https://www.doi.org/10.1021/je400838e
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Effects of Different Organic Acids on Solubility and Metastable Zone Width of Zinc Lactate:	https://www.doi.org/10.1021/je3006453
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77929&Units=SI
Extraction of Citric Acid and Maleic Acid from Their Aqueous Solutions Using a Phosphorus-Bonded Extractant, Tri-n-octylphosphineoxide, and a Secondary Amine, Dioctylamine:	https://www.doi.org/10.1021/acs.jced.7b00562
Influence of Urea on Shifting Hydrophilic to Hydrophobic Interactions of Pr(NO3)3, Sm(NO3)3, and Gd(NO3)3 with BSA in Aqueous Citric Acid: A Volumetric, Viscometric, and Surface Tension Study:	https://www.doi.org/10.1021/je5005388
Influence of temperature, water content and type of organic acid on the formation, stability and properties of functional natural deep eutectic solvents:	https://www.doi.org/10.1016/j.fluid.2019.01.025
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Investigation on Molecular Interactions of Nicotinamide in Aqueous Citric Acid Solutions with Reference to Manifestation of Partial Molar Volume and Viscosity B-Coefficient Measurements:	https://www.doi.org/10.1016/j.tca.2010.05.014
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Experimental Data of Citric Acid Extraction from Aqueous Solution with 1-Decanol by Using Liquid-Liquid Equilibrium:	https://www.doi.org/10.1021/acs.jced.7b01135

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume