Propanedioic acid

Other names:	CARBOXYACETIC ACID
	CH2(COOH)2
	DICARBOXYMETHANE
	Kyselina malonova
	MALONIC ACID
	Methanedicarbonic acid
	Methanedicarboxylic acid
	NSC 8124
	USAF EK-695
Inchi:	InChI=1S/C3H4O4/c4-2(5)1-3(6)7/h1H2,(H,4,5)(H,6,7)
InchiKey:	OFOBLEOULBTSOW-UHFFFAOYSA-N
Formula:	C3H4O4
SMILES:	O=C(O)CC(=O)O
Mol. weight [g/mol]:	104.06
CAS:	141-82-2

Physical Properties

Property code	Value	Unit	Source
chs	-861.57 ± 0.63	kJ/mol	NIST Webbook
chs	-861.15 ± 0.63	kJ/mol	NIST Webbook
gf	-557.10	kJ/mol	Joback Method
hf	-634.87	kJ/mol	Joback Method
hfs	-891.10 ± 0.40	kJ/mol	NIST Webbook
hfus	14.90	kJ/mol	Joback Method
hsub	111.40 ± 0.70	kJ/mol	NIST Webbook
hsub	105.10 ± 0.80	kJ/mol	NIST Webbook
hvap	69.12	kJ/mol	Joback Method
ie	11.05	eV	NIST Webbook
log10ws	0.72		Crippen Method
logp	-0.454		Crippen Method
mcvol	68.010	ml/mol	McGowan Method
pc	6990.97	kPa	Joback Method
ss	149.00	J/mol×K	NIST Webbook
tb	560.14	K	Joback Method
tc	737.52	K	Joback Method
tf	407.90 ± 0.30	K	NIST Webbook
tf	408.05 ± 0.30	K	NIST Webbook

vc	0.254	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.19	J/mol×K	737.52	Joback Method
cpg	166.05	J/mol×K	707.95	Joback Method
cpg	147.44	J/mol×K	560.14	Joback Method
cpg	151.57	J/mol×K	589.70	Joback Method
cpg	155.48	J/mol×K	619.27	Joback Method
cpg	159.20	J/mol×K	648.83	Joback Method
cpg	162.72	J/mol×K	678.39	Joback Method
cps	127.63	J/mol×K	298.15	NIST Webbook
dvisc	0.0001310	Pa×s	524.30	Joback Method
dvisc	0.0000754	Pa×s	560.14	Joback Method
dvisc	0.0115826	Pa×s	345.07	Joback Method
dvisc	0.0033725	Pa×s	380.92	Joback Method
dvisc	0.0012142	Pa×s	416.76	Joback Method
dvisc	0.0005139	Pa×s	452.61	Joback Method
dvisc	0.0002468	Pa×s	488.45	Joback Method
hfust	23.10	kJ/mol	407.50	NIST Webbook
hsubt	72.70	kJ/mol	305.50	NIST Webbook
hsubt	108.90 ± 0.70	kJ/mol	348.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.07123e+01
Coeff. B	-3.47121e+03
Coeff. C	-9.03390e+01
Temperature range (K), min.	423.32
Temperature range (K), max.	733.06

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.11442e+01
Coeff. B	-8.74805e+03
Coeff. C	-2.54993e-03
Coeff. D	4.32749e-09
Temperature range (K), min.	291.15
Temperature range (K), max.	320.15

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=960
Henry s constant of carbon dioxide-aqueous deep eutectic solvent (choline chloride/ethylene glycol, choline chloride/glycerol, choline chloride/malonic acid) systems:	https://www.doi.org/10.1016/j.jct.2013.08.029
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C141822&Units=SI
Fixed-Path Length Laser-Induced Sound Pinging: A Streamlined Method for Sound Speed Determination in Binary Liquids:	https://www.doi.org/10.1021/acs.jced.9b00436
Experimental determination and correlation of acetaminophen solubility in binary eutectic solvents:	https://www.doi.org/10.1016/j.fluid.2018.01.017
Viscosities and Densities of Binary Mixtures of Choline Chloride-Based Deep Eutectic Solvents with Methanol at Various Temperatures:	https://www.doi.org/10.1021/je050366x
Oxalic, Malonic, Succinic, Maleic, Malic, and Tartaric Acids:	https://www.doi.org/10.1016/j.jct.2018.11.019
Liquid–liquid equilibrium of alcohol-ester systems with deep eutectic solvent on the base of choline chloride + malonic acid:	https://www.doi.org/10.1016/j.tca.2014.11.028
Densities of aqueous mixtures of (choline chloride + ethylene glycol) and (choline chloride + malonic acid) deep eutectic solvents in temperature range 283.15–363.15 K:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
The Yaws Handbook of Vapor Pressure:	https://www.doi.org/10.1021/acs.jced.5b00989
Molar Heat Capacity of Selected Type III Deep Eutectic Solvents :	https://www.doi.org/10.1016/j.jct.2016.10.002
Molar enthalpy of mixing and refractive indices of choline chloride-based deep eutectic solvents with water:	https://www.doi.org/10.1021/acs.jced.8b00972
Experimental Study on Reactive Extraction of Malonic Acid with Validation by Fourier Transform Infrared Spectroscopy:	https://www.doi.org/10.1021/je700042z
Mutual Diffusion Coefficients for Binary Aqueous Solutions of Arsenous, Arsenic, and Malonic Acids:	https://www.doi.org/10.1016/j.fluid.2011.09.033
Solubility and structure analysis of malonic and malic acids in different solvents from 303.2 to 333.2 K:	
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
An odd-even effect on solubility of dicarboxylic acids in organic solvents:	https://www.doi.org/10.1016/j.jct.2014.05.009
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
Volumetric properties of aqueous solutions of malonic acid:	https://www.doi.org/10.1016/j.jct.2016.06.023
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=960
Vapor pressure of aqueous choline chloride-based deep eutectic solvents (ethaline, glyceline, maline and reline) at 30 to 70 deg C:	https://www.doi.org/10.1016/j.tca.2012.05.031

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
pvap:	Vapor 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