Oxalic acid

Other names:	Acide oxalique
	Acido ossalico
	Aktisal
	Aquisal
	Ethane-1,2-dioic acid
	Ethanedioic acid
	Ethanedionic acid
	HOOCCOOH
	Kyselina stavelova
	NCI-C55209
	NSC 62774
	Oxaalzuur
	Oxalsaeure
	Oxiric acid
Inchi:	InChI=1S/C2H2O4/c3-1(4)2(5)6/h(H,3,4)(H,5,6)
InchiKey:	MUBZPKHOEPUJKR-UHFFFAOYSA-N
Formula:	C2H2O4
SMILES:	O=C(O)C(=O)O
Mol. weight [g/mol]:	90.03
CAS:	144-62-7

Physical Properties

Property code	Value	Unit	Source
chs	-242.90 ± 0.92	kJ/mol	NIST Webbook
chs	-253.50 ± 0.46	kJ/mol	NIST Webbook
gf	-565.52	kJ/mol	Joback Method
hf	-614.23	kJ/mol	Joback Method
hfs	-828.93 ± 0.46	kJ/mol	NIST Webbook
hfs	-829.94 ± 0.96	kJ/mol	NIST Webbook
hfus	12.31	kJ/mol	Joback Method
hsub	97.91	kJ/mol	NIST Webbook
hvap	66.90	kJ/mol	Joback Method
ie	11.20	eV	NIST Webbook
ie	11.20	eV	NIST Webbook
ie	11.20	eV	NIST Webbook
log10ws	0.38		Aqueous Solubility Prediction Method

logp	-0.844		Crippen Method
mcvol	53.920	ml/mol	McGowan Method
pc	8264.46	kPa	Joback Method
rinpol	748.00		NIST Webbook
ss	115.60	J/mol×K	NIST Webbook
tb	537.26	K	Joback Method
tc	716.26	K	Joback Method
tf	464.45 ± 1.50	K	NIST Webbook
tf	374.65	K	Aqueous Solubility Prediction Method
vc	0.198	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	107.84	J/mol×K	537.26	Joback Method
cpg	110.79	J/mol×K	567.09	Joback Method
cpg	113.60	J/mol×K	596.93	Joback Method
cpg	116.25	J/mol×K	626.76	Joback Method
cpg	118.76	J/mol×K	656.60	Joback Method
cpg	121.13	J/mol×K	686.43	Joback Method
cpg	123.35	J/mol×K	716.26	Joback Method
cps	105.90	J/mol×K	298.15	NIST Webbook
cps	146.00	J/mol×K	340.00	NIST Webbook
cps	118.00	J/mol×K	323.00	NIST Webbook
cps	120.10	J/mol×K	298.10	NIST Webbook
dvisc	0.0143582	Pa×s	333.80	Joback Method
dvisc	0.0042222	Pa×s	367.71	Joback Method
dvisc	0.0015266	Pa×s	401.62	Joback Method
dvisc	0.0006467	Pa×s	435.53	Joback Method
dvisc	0.0003102	Pa×s	469.44	Joback Method
dvisc	0.0001642	Pa×s	503.35	Joback Method
dvisc	0.0000942	Pa×s	537.26	Joback Method
hsubt	61.80	kJ/mol	306.00	NIST Webbook
hsubt	90.60	kJ/mol	355.50	NIST Webbook

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.20464e+01
Coeff. B	-3.82034e+03
Coeff. C	-1.23938e+02
Temperature range (K), min.	448.83
Temperature range (K), max.	691.18

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.87705e+02
Coeff. B	-1.97651e+04
Coeff. C	-2.37488e+01
Coeff. D	7.12656e-06
Temperature range (K), min.	462.65
Temperature range (K), max.	804.00

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Comparison of Extractability of Oxalic Acid from Dilute Aqueous Solutions Using Dioctylamine and Tributylphosphine Oxide: https://www.doi.org/10.1021/acs.jced.8b01155

Effect of Hydrogen Bond Donor on the Physical Properties of Benzyltriethylammonium 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

Density, transport properties and electrochemical potential windows for the 2-hydroxy-N,N,N-trimethylethanaminium chlorides based ionic liquids at several temperatures.: https://www.doi.org/10.1016/j.fluid.2015.03.025

An odd-even effect on solubility of dicarboxylic acids in organic solvents: https://www.doi.org/10.1016/j.jct.2014.05.009

Molar Heat Capacity of Selected Type III Deep Eutectic Solvents : https://www.doi.org/10.1021/acs.jced.5b00989

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C144627&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=959

Experimental determination and correlation of acetaminophen solubility in aqueous solutions of choline chloride based deep eutectic solvents at various temperatures: https://www.doi.org/10.1016/j.fluid.2018.01.017

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=959

Surface Tensions and Densities of Oxalic, Malonic, Succinic, Maleic, Malic, and cis-Pinonic Acids: https://www.doi.org/10.1021/je050366x

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
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
rinpol:	Non-polar retention indices
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume