Ethanedioic acid

Other names:	Acide oxalique
	Acido ossalico
	Aktisal
	Aquisal
	Ethane-1,2-dioic acid
	Ethanedionic acid
	HOOCCOOH
	Kyselina stavelova
	NCI-C55209
	NSC 62774
	Oxaalzuur
	Oxalsaeure
	Oxiric acid
	oxalic 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
af	0.7636		Cheméo Relay (1.0)
chs	-253.50 ± 0.46	kJ/mol	NIST Webbook
chs	-242.90 ± 0.92	kJ/mol	NIST Webbook
gf	-565.52	kJ/mol	Joback Method
hf	-727.93	kJ/mol	Cheméo Relay (1.0)
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	73.86	kJ/mol	Cheméo Relay (1.0)
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	475.23	K	Cheméo Relay (1.0)
tc	707.67	K	Cheméo Relay (1.0)
tf	464.45 ± 1.50	K	NIST Webbook
tf	464.45 ± 1.50	K	NIST Webbook
tf	374.65	K	Aqueous Solubility Prediction Method
vc	0.196	m3/kmol	Cheméo Relay (1.0)

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	146.00	J/mol×K	340.00	NIST Webbook
cps	105.90	J/mol×K	298.15	NIST Webbook
cps	118.00	J/mol×K	323.00	NIST Webbook
cps	120.10	J/mol×K	298.10	NIST Webbook
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
dvisc	0.0143582	Pa×s	333.80	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

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

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

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

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

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

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

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

Cheméo Relay (1.0, beta):

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

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

Cheméo Relay (1.0):

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

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

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

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

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

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

Legend

af:	Acentric Factor
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