Ethanedioic acid, diethyl ester

Other names:	C2H5OCOCOOC2H5
	DIETHYL ESTER OXALIC ACID
	DIETHYL ETHANEDIOATE
	DIETHYL OXALATE
	Diethyl ester of oxalic acid
	Diethylester kyseliny stavelove
	Ethanedioic acid, 1,2-diethyl ester
	Ethyl oxalate
	NSC 8851
	Oxalic acid, diethyl ester
	Oxalic ether
	UN 2525
Inchi:	InChI=1S/C6H10O4/c1-3-9-5(7)6(8)10-4-2/h3-4H2,1-2H3
InchiKey:	WYACBZDAHNBPPB-UHFFFAOYSA-N
Formula:	C6H10O4
SMILES:	CCOC(=O)C(=O)OCC
Mol. weight [g/mol]:	146.14
CAS:	95-92-1

Physical Properties

Property code	Value	Unit	Source
chl	-2981.30	kJ/mol	NIST Webbook
chl	-2984.70 ± 8.40	kJ/mol	NIST Webbook
gf	-468.20	kJ/mol	Joback Method
hf	-656.77	kJ/mol	Joback Method
hfl	-809.73	kJ/mol	NIST Webbook
hfl	-807.72	kJ/mol	NIST Webbook
hfus	16.87	kJ/mol	Joback Method
hvap	47.26	kJ/mol	Joback Method
ie	9.80	eV	NIST Webbook
ie	10.19	eV	NIST Webbook
log10ws	-0.06		Crippen Method
logp	0.113		Crippen Method
mcvol	110.280	ml/mol	McGowan Method
pc	2140.00 ± 4.00	kPa	NIST Webbook

pc	3060.00	kPa	Critical Point and Vapor Pressure Measurements for 17 Compounds by a Low Residence Time Flow Method
rhoc	323.26 ± 2.92	kg/m3	NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	938.00		NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	940.00		NIST Webbook
ripol	1496.00		NIST Webbook
ripol	1530.00		NIST Webbook
tb	458.80 ± 0.30	K	NIST Webbook
tb	458.90	K	NIST Webbook
tb	458.85 ± 1.50	K	NIST Webbook
tb	458.80 ± 0.25	K	NIST Webbook
tb	458.15 ± 0.30	K	NIST Webbook
tc	618.00 ± 2.00	K	NIST Webbook
tf	232.55 ± 0.40	K	NIST Webbook
tf	232.35 ± 0.50	K	NIST Webbook
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.74	J/mol×K	645.76	Joback Method
cpg	263.35	J/mol×K	583.16	Joback Method
cpg	287.43	J/mol×K	677.07	Joback Method
cpg	245.69	J/mol×K	520.56	Joback Method
cpg	236.42	J/mol×K	489.26	Joback Method
cpg	254.67	J/mol×K	551.86	Joback Method
cpg	271.71	J/mol×K	614.46	Joback Method
cpl	260.70	J/mol×K	298.00	NIST Webbook
dvisc	0.0014800	Pa×s	308.15	Densities, Viscosities, and Refractive Indices of Binary Mixtures of Diethyl Oxalate with Some Ketones at (303.15, 308.15, and 313.15) K

dvisc	0.0013670	Pa×s	313.15	Densities, Viscosities, and Refractive Indices of Binary Mixtures of Diethyl Oxalate with Some Ketones at (303.15, 308.15, and 313.15) K
dvisc	0.0016230	Pa×s	303.15	Densities, Viscosities, and Refractive Indices of Binary Mixtures of Diethyl Oxalate with Some Ketones at (303.15, 308.15, and 313.15) K
hvapt	53.90	kJ/mol	400.00	NIST Webbook
hvapt	62.30	kJ/mol	389.50	NIST Webbook
pvap	0.38	kPa	325.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.48	kPa	329.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.63	kPa	333.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.24	kPa	318.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.13	kPa	308.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids

pvap	0.15	kPa	311.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.17	kPa	313.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.21	kPa	316.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.02	kPa	283.60	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.03	kPa	288.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.04	kPa	293.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.06	kPa	298.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	

pvap	0.08	kPa	303.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.30	kPa	321.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
rfi	1.40340		308.15	Density, Viscosity, Refractive Index, and Speed of Sound in the Binary Mixtures of 1,4-Dioxane + Ethyl Acetoacetate, + Diethyl Oxalate, + Diethyl Phthalate, or + Dioctyl Phthalate at 298.15, 303.15, and 308.15 K
rfi	1.40840		298.15	Density, Viscosity, Refractive Index, and Speed of Sound for Binary Mixtures of Anisole with 2-Chloroethanol, 1,4-Dioxane, Tetrachloroethylene, Tetrachloroethane, DMF, DMSO, and Diethyl Oxalate at (298.15, 303.15, and 308.15) K
rfi	1.40610		303.15	Density, Viscosity, Refractive Index, and Speed of Sound for Binary Mixtures of Anisole with 2-Chloroethanol, 1,4-Dioxane, Tetrachloroethylene, Tetrachloroethane, DMF, DMSO, and Diethyl Oxalate at (298.15, 303.15, and 308.15) K

rfi	1.40390		308.15	Density, Viscosity, Refractive Index, and Speed of Sound for Binary Mixtures of Anisole with 2-Chloroethanol, 1,4-Dioxane, Tetrachloroethylene, Tetrachloroethane, DMF, DMSO, and Diethyl Oxalate at (298.15, 303.15, and 308.15) K
rfi	1.40600		303.15	Density, Viscosity, Refractive Index, and Speed of Sound in the Binary Mixtures of 1,4-Dioxane + Ethyl Acetoacetate, + Diethyl Oxalate, + Diethyl Phthalate, or + Dioctyl Phthalate at 298.15, 303.15, and 308.15 K
rfi	1.40840		298.15	Density, Viscosity, Refractive Index, and Speed of Sound in the Binary Mixtures of 1,4-Dioxane + Ethyl Acetoacetate, + Diethyl Oxalate, + Diethyl Phthalate, or + Dioctyl Phthalate at 298.15, 303.15, and 308.15 K
rhol	1095.94	kg/m3	278.15	Excess molar enthalpies of {diethyl oxalate + (methanol, + ethanol, + 1-propanol, and + 2-propanol)} at T = (288.2, 298.2, 313.2, and 328.2) K and p = 101.3 kPa

rhol	1001.60	kg/m3	358.15	Excess molar enthalpies of {diethyl oxalate + (methanol, + ethanol, + 1-propanol, and + 2-propanol)} at T = (288.2, 298.2, 313.2, and 328.2) K and p = 101.3 kPa
rhol	1013.53	kg/m3	348.15	Excess molar enthalpies of {diethyl oxalate + (methanol, + ethanol, + 1-propanol, and + 2-propanol)} at T = (288.2, 298.2, 313.2, and 328.2) K and p = 101.3 kPa
rhol	1037.26	kg/m3	328.15	Excess molar enthalpies of {diethyl oxalate + (methanol, + ethanol, + 1-propanol, and + 2-propanol)} at T = (288.2, 298.2, 313.2, and 328.2) K and p = 101.3 kPa
rhol	1054.92	kg/m3	313.15	Excess molar enthalpies of {diethyl oxalate + (methanol, + ethanol, + 1-propanol, and + 2-propanol)} at T = (288.2, 298.2, 313.2, and 328.2) K and p = 101.3 kPa
rhol	1072.53	kg/m3	298.15	Excess molar enthalpies of {diethyl oxalate + (methanol, + ethanol, + 1-propanol, and + 2-propanol)} at T = (288.2, 298.2, 313.2, and 328.2) K and p = 101.3 kPa

rhol	1084.24	kg/m3	288.14	Excess molar enthalpies of {diethyl oxalate + (methanol, + ethanol, + 1-propanol, and + 2-propanol)} at T = (288.2, 298.2, 313.2, and 328.2) K and p = 101.3 kPa
rhol	1025.42	kg/m3	338.15	Excess molar enthalpies of {diethyl oxalate + (methanol, + ethanol, + 1-propanol, and + 2-propanol)} at T = (288.2, 298.2, 313.2, and 328.2) K and p = 101.3 kPa

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	370.20	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62354e+01
Coeff. B	-4.44264e+03
Coeff. C	-7.61870e+01
Temperature range (K), min.	354.76
Temperature range (K), max.	482.88

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.25933e+02
Coeff. B	-1.13116e+04

Coeff. C	-1.60682e+01
Coeff. D	8.62399e-06
Temperature range (K), min.	232.55
Temperature range (K), max.	646.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Density, Viscosity, Refractive Index, and Speed of Sound for Binary Mixtures of Anisole with 2-Chloroethanol, 1,4-Dioxane, Tetrachloroethylene, Tetrachloroethane, DMF, DMSO, and Diethyl Oxalate at (298.15, 303.15, and 308.15) K:	https://www.doi.org/10.1021/je049610v
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Density, Viscosity, Refractive Index, and Speed of Sound in the Binary Mixtures of 1,4-Dioxane + Ethyl Acetoacetate, + Diethyl Oxalate, + Diethyl Phthalate, or + Dioctyl Phthalate at 298.15, 303.15, and 308.15 K:	https://www.doi.org/10.1021/je0301489
Critical Point and Vapor Pressure Measurements for 17 Compounds by a Low Residence Time Flow Method:	https://www.doi.org/10.1021/je060269j
Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids:	https://www.doi.org/10.1021/je100231g
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1074
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95921&Units=SI
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1074.mol
Densities, Viscosities, and Refractive Indices of Binary Mixtures of Diethyl Oxalate with Some Ketones at (303.15, 308.15, and 313.15) K:	https://www.doi.org/10.1021/je100715x
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Excess molar enthalpies of {diethyl oxalate + (methanol, + ethanol, + 1-propanol, and + 2-propanol)} at T = (288.2, 298.2, 313.2, and 328.2) K and p = 101.3 kPa:	https://www.doi.org/10.1016/j.jct.2013.05.024
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
rfi:	Refractive Index
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume