Diethyl malonate

Other names:	1,3-propanedioic acid, diethyl ester
	Carbethoxyacetic ester
	Dicarbethoxymethane
	Diethyl propanedioate
	Ethyl malonate
	Malonic acid diethylester
	Malonic acid, diethyl ester
	Malonic ester
	Methanedicarboxylic acid, diethyl ester
	NSC 8864
	Propanedioic acid, 1,3-diethyl ester
	Propanedioic acid, diethyl ester
	diethyl 1,3-propanedioate
Inchi:	InChI=1S/C7H12O4/c1-3-10-6(8)5-7(9)11-4-2/h3-5H2,1-2H3
InchiKey:	IYXGSMUGOJNHAZ-UHFFFAOYSA-N
Formula:	C7H12O4
SMILES:	CCOC(=O)CC(=O)OCC
Mol. weight [g/mol]:	160.17
CAS:	105-53-3

Physical Properties

Property code	Value	Unit	Source
chl	-3483.00 ± 4.10	kJ/mol	NIST Webbook
gf	-459.78	kJ/mol	Joback Method
hf	-921.70 ± 4.20	kJ/mol	NIST Webbook
hfl	-986.60 ± 4.20	kJ/mol	NIST Webbook
hfus	19.46	kJ/mol	Joback Method
hvap	64.90	kJ/mol	NIST Webbook
hvap	64.70 ± 0.20	kJ/mol	NIST Webbook
log10ws	-0.82		Aqueous Solubility Prediction Method
log10ws	-0.82		Estimated Solubility Method
logp	0.503		Crippen Method
mcvol	124.370	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
rinpol	1069.20		NIST Webbook

rinpol	1038.00	NIST Webbook
rinpol	1033.00	NIST Webbook
rinpol	1033.30	NIST Webbook
rinpol	1033.00	NIST Webbook
rinpol	1083.00	NIST Webbook
rinpol	1038.00	NIST Webbook
rinpol	1068.80	NIST Webbook
rinpol	1069.20	NIST Webbook
rinpol	1034.00	NIST Webbook
rinpol	1035.00	NIST Webbook
rinpol	1066.90	NIST Webbook
rinpol	1069.00	NIST Webbook
rinpol	1034.00	NIST Webbook
rinpol	1034.00	NIST Webbook
rinpol	1032.00	NIST Webbook
rinpol	1029.00	NIST Webbook
rinpol	1033.00	NIST Webbook
rinpol	1069.00	NIST Webbook
rinpol	1032.00	NIST Webbook
rinpol	1069.00	NIST Webbook
rinpol	1072.00	NIST Webbook
rinpol	1043.00	NIST Webbook
rinpol	1043.00	NIST Webbook
rinpol	1064.00	NIST Webbook
rinpol	1040.00	NIST Webbook
rinpol	1035.00	NIST Webbook
rinpol	1078.00	NIST Webbook
rinpol	1069.00	NIST Webbook
rinpol	1040.00	NIST Webbook
rinpol	1066.90	NIST Webbook
rinpol	1078.00	NIST Webbook
ripol	1595.00	NIST Webbook
ripol	1574.00	NIST Webbook
ripol	1580.00	NIST Webbook
ripol	1595.00	NIST Webbook
ripol	1580.00	NIST Webbook
ripol	1572.00	NIST Webbook
ripol	1574.00	NIST Webbook
ripol	1571.00	NIST Webbook
ripol	1571.00	NIST Webbook
ripol	1572.00	NIST Webbook
ripol	1572.00	NIST Webbook
ripol	1582.00	NIST Webbook
ripol	1542.00	NIST Webbook

ripol	1572.00		NIST Webbook
ripol	1574.00		NIST Webbook
tb	472.05 ± 0.30	K	NIST Webbook
tb	373.35 ± 0.40	K	NIST Webbook
tb	472.50	K	NIST Webbook
tb	473.05	K	Ternary phase diagrams for aqueous mixtures of butyric acid with several solvents: experimental and correlated data
tc	651.00	K	Critical temperatures and pressures of some dicarboxylic acid diethyl esters
tf	224.30 ± 1.00	K	NIST Webbook
tf	221.70 ± 0.50	K	NIST Webbook
tf	223.25 ± 0.30	K	NIST Webbook
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.74	J/mol×K	543.09	Joback Method
cpg	298.81	J/mol×K	574.05	Joback Method
cpg	308.51	J/mol×K	605.00	Joback Method
cpg	317.83	J/mol×K	635.96	Joback Method
cpg	326.76	J/mol×K	666.91	Joback Method
cpg	278.30	J/mol×K	512.14	Joback Method
cpg	335.29	J/mol×K	697.87	Joback Method
cpl	300.20	J/mol×K	298.15	NIST Webbook
cpl	284.90	J/mol×K	294.60	NIST Webbook
cpl	284.90	J/mol×K	294.60	NIST Webbook
dvisc	0.0020676	Pa×s	312.97	Joback Method
dvisc	0.0012258	Pa×s	346.17	Joback Method
dvisc	0.0007964	Pa×s	379.36	Joback Method
dvisc	0.0002482	Pa×s	512.14	Joback Method
dvisc	0.0005546	Pa×s	412.56	Joback Method
dvisc	0.0004076	Pa×s	445.75	Joback Method
dvisc	0.0003126	Pa×s	478.94	Joback Method
hvapt	51.20	kJ/mol	392.50	NIST Webbook
hvapt	63.30	kJ/mol	305.50	NIST Webbook
hvapt	64.70 ± 0.20	kJ/mol	303.00	NIST Webbook
hvapt	59.90	kJ/mol	426.00	NIST Webbook

pvap	3.38e-03	kPa	272.85	Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl Malonate
pvap	5.46e-03	kPa	277.85	Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl Malonate
pvap	4.46e-03	kPa	276.75	Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl Malonate
pvap	7.97e-03	kPa	282.85	Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl Malonate
pvap	9.15e-03	kPa	284.55	Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl Malonate
pvap	0.01	kPa	287.95	Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl Malonate
pvap	4.36e-03	kPa	275.65	Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl Malonate
pvap	6.37e-03	kPa	279.85	Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl Malonate
pvap	3.28e-03	kPa	274.15	Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl Malonate
pvap	2.55e-03	kPa	271.65	Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl Malonate
pvap	2.41e-03	kPa	270.55	Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl Malonate
pvap	1.94e-03	kPa	269.05	Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl Malonate

pvap	1.89e-03	kPa	267.65	Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl Malonate	
pvap	1.44e-03	kPa	265.15	Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl Malonate	
pvap	0.10	kPa	316.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.08	kPa	313.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.06	kPa	310.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.05	kPa	307.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.04	kPa	304.70	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.04	kPa	304.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	

pvap	0.03	kPa	301.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.02	kPa	295.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.01	kPa	292.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.01	kPa	289.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	8.58e-03	kPa	286.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.03	kPa	298.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	6.89e-03	kPa	283.80	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	

rfi	1.40850		308.15	Density, Viscosity, Refractive Index, and Speed of Sound for Binary Mixtures of 1,4-Dioxane with Different Organic Liquids at (298.15, 303.15, and 308.15) K
rfi	1.41400		293.15	Bubble points measurement for (triethyl orthoformate + diethyl malonate)
rfi	1.41320		298.15	Density, Viscosity, Refractive Index, and Speed of Sound for Binary Mixtures of 1,4-Dioxane with Different Organic Liquids at (298.15, 303.15, and 308.15) K
rfi	1.41080		303.15	Density, Viscosity, Refractive Index, and Speed of Sound for Binary Mixtures of 1,4-Dioxane with Different Organic Liquids at (298.15, 303.15, and 308.15) K
rhol	995.63	kg/m3	348.15	Excess Molar Enthalpies of Diethyl Malonate + (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	1049.60	kg/m3	298.15	Excess Molar Enthalpies of Diethyl Malonate + (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	1060.33	kg/m3	288.14	Excess Molar Enthalpies of Diethyl Malonate + (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	1071.04	kg/m3	278.15	Excess Molar Enthalpies of Diethyl Malonate + (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	1017.34	kg/m3	328.15	Excess Molar Volumes of 1,3-Diethyl Propanedioate with Methanol, Ethanol, Propan-1-ol, Propan-2-ol, Butan-2-ol, 2-Methyl-propan-1-ol, and Pentan-1-ol at T = (288.15, 298.15, 313.15, and 328.15) K
rhol	1033.50	kg/m3	313.15	Excess Molar Volumes of 1,3-Diethyl Propanedioate with Methanol, Ethanol, Propan-1-ol, Propan-2-ol, Butan-2-ol, 2-Methyl-propan-1-ol, and Pentan-1-ol at T = (288.15, 298.15, 313.15, and 328.15) K
rhol	1049.60	kg/m3	298.15	Excess Molar Volumes of 1,3-Diethyl Propanedioate with Methanol, Ethanol, Propan-1-ol, Propan-2-ol, Butan-2-ol, 2-Methyl-propan-1-ol, and Pentan-1-ol at T = (288.15, 298.15, 313.15, and 328.15) K

rhol	1060.33	kg/m3	288.15	Excess Molar Volumes of 1,3-Diethyl Propanedioate with Methanol, Ethanol, Propan-1-ol, Propan-2-ol, Butan-2-ol, 2-Methyl-propan-1-ol, and Pentan-1-ol at T = (288.15, 298.15, 313.15, and 328.15) K
rhol	1055.25	kg/m3	293.20	Modeling extraction equilibria of butyric acid distributed between water and tri-n-butyl amine/diluent or tri-n-butyl phosphate/diluent system: Extension of the LSER approach
rhol	995.63	kg/m3	348.15	Excess molar enthalpies of diethyl malonate+ (1-butanol, 2-methyl-1-propanol, 1-pentanol, n-heptane, and ethyl acetate) at T= (288.2, 298.2, 313.2, 328.2, 338.2, and 348.2 K) and p = 101.3 kPa
rhol	1017.34	kg/m3	328.15	Excess molar enthalpies of diethyl malonate+ (1-butanol, 2-methyl-1-propanol, 1-pentanol, n-heptane, and ethyl acetate) at T= (288.2, 298.2, 313.2, 328.2, 338.2, and 348.2 K) and p = 101.3 kPa

rhol	1033.50	kg/m3	313.15	Excess molar enthalpies of diethyl malonate+ (1-butanol, 2-methyl-1-propanol, 1-pentanol, n-heptane, and ethyl acetate) at T= (288.2, 298.2, 313.2, 328.2, 338.2, and 348.2 K) and p = 101.3 kPa
rhol	1049.60	kg/m3	298.15	Excess molar enthalpies of diethyl malonate+ (1-butanol, 2-methyl-1-propanol, 1-pentanol, n-heptane, and ethyl acetate) at T= (288.2, 298.2, 313.2, 328.2, 338.2, and 348.2 K) and p = 101.3 kPa
rhol	1060.33	kg/m3	288.15	Excess molar enthalpies of diethyl malonate+ (1-butanol, 2-methyl-1-propanol, 1-pentanol, n-heptane, and ethyl acetate) at T= (288.2, 298.2, 313.2, 328.2, 338.2, and 348.2 K) and p = 101.3 kPa
rhol	1033.50	kg/m3	313.15	Excess Molar Enthalpies of Diethyl Malonate + (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	1017.34	kg/m3	328.15	Excess Molar Enthalpies of Diethyl Malonate + (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	1006.50	kg/m3	338.15	Excess Molar Enthalpies of Diethyl Malonate + (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	984.70	kg/m3	358.15	Excess Molar Enthalpies of Diethyl Malonate + (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	1006.50	kg/m3	338.15	Excess molar enthalpies of diethyl malonate+ (1-butanol, 2-methyl-1-propanol, 1-pentanol, n-heptane, and ethyl acetate) at T= (288.2, 298.2, 313.2, 328.2, 338.2, and 348.2 K) and p = 101.3 kPa

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.36189e+00
Coeff. B	-5.71086e+03
Coeff. C	1.55030e+00
Coeff. D	-8.41809e-07
Temperature range (K), min.	313.15
Temperature range (K), max.	472.15

Datasets

Viscosity, Pa*s

Temperature, K - Liquid	Pressure, kPa - Liquid	Viscosity, Pa*s - Liquid
303.15	101.30	0.0017210

Reference *https://www.doi.org/10.1016/j.tca.2004.07.014*

Sources

Critical temperatures and pressures of some dicarboxylic acid diethyl esters:	https://www.doi.org/10.1016/j.fluid.2015.12.031
Modeling extraction equilibria of butyric acid distributed between water and tri-n-butyl amine/diluent or tri-n-butyl phosphate/diluent system: Extension of the LSER approach:	https://www.doi.org/10.1016/j.fluid.2014.10.043
Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl	https://www.doi.org/10.1021/je500428d
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
Excess molar enthalpies of diethyl malonate + (1-butanol, 2-methyl-1-propanol, 1-pentanol, n-heptane, and ethyl acetate) at T = (288.2, 298.2, 313.2, 328.2, 338.2, and	https://www.doi.org/10.1016/j.fluid.2009.11.030
Excess Molar Volumes of 1,3-Diethyl Propanedioate with Methanol, Ethanol, Propan-1-ol, Propan-2-ol, Butan-2-ol, 2-Methyl-propan-1-ol, and Pentan-1-ol at T = (288.15, 298.15, 313.15, and 328.15) K:	https://www.doi.org/10.1021/je100100n
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Ternary phase diagrams for aqueous mixtures of butyric acid with several solvents: experimental and correlated data:	https://www.doi.org/10.1016/j.fluid.2014.03.008
Extraction of propionic acid by diethyl carbonate or diethyl malonate or diethyl fumarate and the synergistic effect of phosphorus compounds and amines:	https://www.doi.org/10.1016/j.fluid.2010.01.018
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105533&Units=SI
Bubble points measurement for (triethyl orthoformate + diethyl malonate):	https://www.doi.org/10.1016/j.jct.2004.07.023
Liquid-phase equilibria of (water + formic acid + diethyl carbonate or diethyl malonate or diethyl fumarate) ternary systems at 298.15K and atmospheric pressure:	https://www.doi.org/10.1016/j.fluid.2010.08.030
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Speeds of sound, isentropic compressibilities, viscosities, and excess molar volumes of binary mixtures of alkanoates with tetra- and trichloromethanes at 303.15 K:	https://www.doi.org/10.1016/j.tca.2004.07.014
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Biomass-Derived Platform Chemicals: Thermodynamic Studies on the Extraction of 5-Hydroxymethylfurfural from Ionic Liquids:	https://www.doi.org/10.1021/je300529j
Excess Molar Enthalpies of Diethyl Malonate + (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/10.1021/je9003806
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1085
Density, Viscosity, Refractive Index, and Speed of Sound for Binary Mixtures of 1,4-Dioxane with Different Organic Liquids at (298.15, 303.15, and 308.15) K:	https://www.doi.org/10.1021/je049609w
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume