Diethyl Phthalate

Other names:	1,2-Benzenedicarboxylic acid, 1,2-diethyl ester
	1,2-Benzenedicarboxylic acid, diethyl ester
	1,2-benzenedioic acid, diethyl ester
	1,2-diethyl phthalate
	Anozol
	DEP
	DIETHYL ESTER
	Diethyl ester of 1,2-Benzenedicarboxylic acid
	Diethyl-1,2-benzenedicarboxylate
	Diethyl-o-phthalate
	Diethylester kyseliny ftalove
	Estol 1550
	Ethyl phthalate
	Kodaflex DEP
	NCI-C60048
	NSC 8905
	Neantine
	O-BENZENEDICARBOXYLIC ACID
	Palatinol A
	Phthalic acid, diethyl ester
	Phthalol
	Phthalsaeurediaethylester
	Placidol E
	Rcra waste number U088
	Solvanol
	Unimoll DA
	diethyl 1,2-benzenedicarboxylate
	diethyl 1,2-benzenedioate
	diethyl benzene-1,2-dicarboxylate
	o-Benzenedicarboxylic acid, diethyl ester
	o-Bis(ethoxycarbonyl)benzene
Inchi:	InChI=1S/C12H14O4/c1-3-15-11(13)9-7-5-6-8-10(9)12(14)16-4-2/h5-8H,3-4H2,1-2H3
InchiKey:	FLKPEMZONWLCSK-UHFFFAOYSA-N
Formula:	C12H14O4
SMILES:	CCOC(=O)c1ccccc1C(=O)OCC
Mol. weight [g/mol]:	222.24
CAS:	84-66-2

Physical Properties

Property code	Value	Unit	Source
chl	-6077.65	kJ/mol	NIST Webbook
chl	-5946.00 ± 12.00	kJ/mol	NIST Webbook
chl	-6073.90	kJ/mol	NIST Webbook
ea	0.54	eV	NIST Webbook
gf	-314.90	kJ/mol	Joback Method
hf	-685.00 ± 13.00	kJ/mol	NIST Webbook
hf	-661.40	kJ/mol	NIST Webbook
hfl	-753.08	kJ/mol	NIST Webbook
hfl	-777.00 ± 12.00	kJ/mol	NIST Webbook
hfus	26.06	kJ/mol	Joback Method
hvap	82.10 ± 0.50	kJ/mol	NIST Webbook
hvap	81.10 ± 0.80	kJ/mol	NIST Webbook
hvap	87.40	kJ/mol	NIST Webbook
log10ws	-2.36		Aqueous Solubility Prediction Method
log10ws	-2.35		Estimated Solubility Method
logp	2.040		Crippen Method
mcvol	171.060	ml/mol	McGowan Method
pc	2260.00	kPa	Critical Temperatures and Pressures of 12 Phthalates Using the Pulse-Heating Method
rinpol	1550.90		NIST Webbook
rinpol	1561.87		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1583.00		NIST Webbook
rinpol	1587.00		NIST Webbook
rinpol	1603.00		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1568.00		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1568.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1543.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1547.50		NIST Webbook
rinpol	1550.90		NIST Webbook
rinpol	1558.00		NIST Webbook

rinpol	1584.00	NIST Webbook
rinpol	1562.22	NIST Webbook
rinpol	1563.47	NIST Webbook
rinpol	1561.87	NIST Webbook
rinpol	1570.77	NIST Webbook
rinpol	1572.65	NIST Webbook
rinpol	1569.25	NIST Webbook
rinpol	1563.84	NIST Webbook
rinpol	1567.00	NIST Webbook
rinpol	1568.00	NIST Webbook
rinpol	1558.00	NIST Webbook
rinpol	1546.00	NIST Webbook
rinpol	1549.00	NIST Webbook
rinpol	1595.00	NIST Webbook
rinpol	1583.00	NIST Webbook
rinpol	1594.00	NIST Webbook
rinpol	1559.00	NIST Webbook
rinpol	1546.00	NIST Webbook
rinpol	1602.30	NIST Webbook
rinpol	1545.00	NIST Webbook
rinpol	1546.00	NIST Webbook
rinpol	1547.00	NIST Webbook
rinpol	1550.00	NIST Webbook
rinpol	1578.00	NIST Webbook
rinpol	1578.00	NIST Webbook
rinpol	1578.00	NIST Webbook
rinpol	1578.00	NIST Webbook
rinpol	1578.00	NIST Webbook
rinpol	1579.00	NIST Webbook
rinpol	1582.00	NIST Webbook
rinpol	1585.00	NIST Webbook
rinpol	1541.00	NIST Webbook
rinpol	1556.00	NIST Webbook
rinpol	1563.00	NIST Webbook
rinpol	1597.00	NIST Webbook
rinpol	1551.00	NIST Webbook
rinpol	1547.00	NIST Webbook
rinpol	1559.00	NIST Webbook
rinpol	1601.00	NIST Webbook
rinpol	1591.00	NIST Webbook
rinpol	1592.00	NIST Webbook
rinpol	1567.00	NIST Webbook
rinpol	1610.00	NIST Webbook
rinpol	1546.00	NIST Webbook

rinpol	1610.00	NIST Webbook
rinpol	1583.00	NIST Webbook
rinpol	1595.00	NIST Webbook
rinpol	1603.00	NIST Webbook
rinpol	1570.00	NIST Webbook
rinpol	1597.00	NIST Webbook
rinpol	1583.00	NIST Webbook
rinpol	1565.00	NIST Webbook
rinpol	1548.00	NIST Webbook
rinpol	1551.00	NIST Webbook
rinpol	1559.00	NIST Webbook
rinpol	1564.00	NIST Webbook
rinpol	1560.00	NIST Webbook
rinpol	1563.00	NIST Webbook
rinpol	1604.00	NIST Webbook
rinpol	1564.00	NIST Webbook
rinpol	271.90	NIST Webbook
rinpol	269.90	NIST Webbook
rinpol	271.04	NIST Webbook
rinpol	272.56	NIST Webbook
rinpol	1601.00	NIST Webbook
rinpol	1546.00	NIST Webbook
rinpol	1570.00	NIST Webbook
rinpol	1551.00	NIST Webbook
rinpol	1604.00	NIST Webbook
rinpol	1551.10	NIST Webbook
rinpol	1594.00	NIST Webbook
rinpol	1578.00	NIST Webbook
rinpol	1585.00	NIST Webbook
rinpol	1605.00	NIST Webbook
rinpol	1594.00	NIST Webbook
rinpol	1551.10	NIST Webbook
ripol	2333.00	NIST Webbook
ripol	2311.00	NIST Webbook
ripol	2355.00	NIST Webbook
ripol	2312.00	NIST Webbook
ripol	2311.00	NIST Webbook
ripol	2346.00	NIST Webbook
ripol	2365.00	NIST Webbook
ripol	2366.00	NIST Webbook
ripol	2378.00	NIST Webbook
ripol	2380.00	NIST Webbook
ripol	2309.00	NIST Webbook
ripol	2380.00	NIST Webbook

ripol	2370.00		NIST Webbook
ripol	2401.00		NIST Webbook
ripol	2370.00		NIST Webbook
ripol	2372.00		NIST Webbook
ripol	2366.00		NIST Webbook
ripol	2358.90		NIST Webbook
ripol	2361.10		NIST Webbook
ripol	2319.00		NIST Webbook
ripol	2355.00		NIST Webbook
ripol	2374.00		NIST Webbook
ripol	2346.00		NIST Webbook
ripol	2361.00		NIST Webbook
ripol	2358.00		NIST Webbook
ripol	2365.00		NIST Webbook
ripol	2365.00		NIST Webbook
ripol	2407.00		NIST Webbook
ripol	2400.00		NIST Webbook
ripol	2378.00		NIST Webbook
sl	425.08	J/mol×K	NIST Webbook
tb	562.65	K	KDB
tb	571.20	K	NIST Webbook
tb	571.00	K	NIST Webbook
tb	571.65 ± 1.00	K	NIST Webbook
tb	571.17	K	(Liquid + liquid) equilibria of (water + propionic acid + diethyl phthalate) at several temperatures
tc	870.02	K	Joback Method
tf	272.80	K	NIST Webbook
tf	245.53	K	Aqueous Solubility Prediction Method
tf	240.15 ± 1.00	K	NIST Webbook
tt	269.92 ± 0.02	K	NIST Webbook
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.51	J/mol×K	658.20	Joback Method
cpg	449.86	J/mol×K	693.50	Joback Method
cpg	462.40	J/mol×K	728.81	Joback Method
cpg	474.13	J/mol×K	764.11	Joback Method

cpg	485.06	J/mol×K	799.41	Joback Method
cpg	495.18	J/mol×K	834.72	Joback Method
cpg	504.49	J/mol×K	870.02	Joback Method
cpl	357.70	J/mol×K	298.15	NIST Webbook
cpl	366.15	J/mol×K	298.15	NIST Webbook
dvisc	0.0001863	Pa×s	616.54	Joback Method
dvisc	0.0006814	Pa×s	449.92	Joback Method
dvisc	0.0004537	Pa×s	491.57	Joback Method
dvisc	0.0003219	Pa×s	533.23	Joback Method
dvisc	0.0001492	Pa×s	658.20	Joback Method
dvisc	0.0002401	Pa×s	574.89	Joback Method
dvisc	0.0011118	Pa×s	408.26	Joback Method
hfust	17.99	kJ/mol	269.90	NIST Webbook
hfust	17.99	kJ/mol	269.90	NIST Webbook
hfust	17.98	kJ/mol	269.92	NIST Webbook
hvapt	88.60	kJ/mol	298.00	A Comparison of Results by Correlation Gas Chromatography with Another Gas Chromatographic Retention Time Technique. The Effects of Retention Time Coincidence on Vaporization Enthalpy and Vapor Pressure
hvapt	65.90	kJ/mol	474.00	NIST Webbook
hvapt	88.30 ± 2.10	kJ/mol	233.00	NIST Webbook
hvapt	77.90	kJ/mol	399.00	NIST Webbook
hvapt	74.60	kJ/mol	426.00	NIST Webbook
hvapt	86.80	kJ/mol	320.00	NIST Webbook
hvapt	59.10	kJ/mol	495.50	NIST Webbook
pvap	1.16e-03	kPa	323.04	Vapour pressure of diethyl phthalate
pvap	0.01	kPa	352.20	Apparatus to measure the vapor pressure of slowly decomposing compounds from 1 Pa to 105 Pa
pvap	0.01	kPa	352.18	Apparatus to measure the vapor pressure of slowly decomposing compounds from 1 Pa to 105 Pa

pvap	6.23e-03	kPa	342.19	Apparatus to measure the vapor pressure of slowly decomposing compounds from 1 Pa to 105 Pa
pvap	0.03	kPa	362.20	Apparatus to measure the vapor pressure of slowly decomposing compounds from 1 Pa to 105 Pa
pvap	0.05	kPa	372.19	Apparatus to measure the vapor pressure of slowly decomposing compounds from 1 Pa to 105 Pa
pvap	0.05	kPa	372.20	Apparatus to measure the vapor pressure of slowly decomposing compounds from 1 Pa to 105 Pa
pvap	0.05	kPa	372.22	Apparatus to measure the vapor pressure of slowly decomposing compounds from 1 Pa to 105 Pa
pvap	0.10	kPa	382.23	Apparatus to measure the vapor pressure of slowly decomposing compounds from 1 Pa to 105 Pa
pvap	0.18	kPa	392.24	Apparatus to measure the vapor pressure of slowly decomposing compounds from 1 Pa to 105 Pa
pvap	0.32	kPa	402.37	Apparatus to measure the vapor pressure of slowly decomposing compounds from 1 Pa to 105 Pa
pvap	0.53	kPa	412.38	Apparatus to measure the vapor pressure of slowly decomposing compounds from 1 Pa to 105 Pa

pvap	0.86	kPa	422.49	Apparatus to measure the vapor pressure of slowly decomposing compounds from 1 Pa to 105 Pa
pvap	2.08	kPa	442.28	Apparatus to measure the vapor pressure of slowly decomposing compounds from 1 Pa to 105 Pa
pvap	1.65e-04	kPa	303.19	Vapour pressure of diethyl phthalate
pvap	2.60e-04	kPa	307.62	Vapour pressure of diethyl phthalate
pvap	2.71e-04	kPa	308.10	Vapour pressure of diethyl phthalate
pvap	4.56e-04	kPa	313.34	Vapour pressure of diethyl phthalate
pvap	7.69e-04	kPa	318.54	Vapour pressure of diethyl phthalate
pvap	2.69e-03	kPa	332.21	Apparatus to measure the vapor pressure of slowly decomposing compounds from 1 Pa to 105 Pa
pvap	1.18e-03	kPa	323.33	Vapour pressure of diethyl phthalate
pvap	1.84e-03	kPa	328.33	Vapour pressure of diethyl phthalate
pvap	2.84e-03	kPa	333.55	Vapour pressure of diethyl phthalate
pvap	2.90e-03	kPa	333.58	Vapour pressure of diethyl phthalate
pvap	2.86e-03	kPa	333.68	Vapour pressure of diethyl phthalate
pvap	3.87e-03	kPa	337.65	Vapour pressure of diethyl phthalate
pvap	4.38e-03	kPa	338.68	Vapour pressure of diethyl phthalate

pvap	6.57e-03	kPa	343.70	Vapour pressure of diethyl phthalate
pvap	3.20e-04	kPa	312.21	Apparatus to measure the vapor pressure of slowly decomposing compounds from 1 Pa to 105 Pa
pvap	3.50e-04	kPa	312.21	Apparatus to measure the vapor pressure of slowly decomposing compounds from 1 Pa to 105 Pa
pvap	1.05e-03	kPa	322.21	Apparatus to measure the vapor pressure of slowly decomposing compounds from 1 Pa to 105 Pa
pvap	1.03e-03	kPa	322.21	Apparatus to measure the vapor pressure of slowly decomposing compounds from 1 Pa to 105 Pa
pvap	3.10	kPa	452.12	Apparatus to measure the vapor pressure of slowly decomposing compounds from 1 Pa to 105 Pa
rfi	1.49580		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	1.49780	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	1.48970	323.15	Solubilities of Diethyl Phthalate, Dicyclopentadiene, and Styrene in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate
rfi	1.49170	318.15	Solubilities of Diethyl Phthalate, Dicyclopentadiene, and Styrene in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate
rfi	1.49390	313.15	Solubilities of Diethyl Phthalate, Dicyclopentadiene, and Styrene in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate
rfi	1.49620	308.15	Solubilities of Diethyl Phthalate, Dicyclopentadiene, and Styrene in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate
rfi	1.49840	303.15	Solubilities of Diethyl Phthalate, Dicyclopentadiene, and Styrene in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate
rfi	1.50050	298.15	Solubilities of Diethyl Phthalate, Dicyclopentadiene, and Styrene in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate

rfi	1.50270		293.15	Solubilities of Diethyl Phthalate, Dicyclopentadiene, and Styrene in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate
rfi	1.50480		288.15	Solubilities of Diethyl Phthalate, Dicyclopentadiene, and Styrene in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate
rfi	1.50700		283.15	Solubilities of Diethyl Phthalate, Dicyclopentadiene, and Styrene in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate
rfi	1.50160		293.20	Isobaric (vapor + liquid) equilibria of the binary system maleic anhydride and diethyl phthalate at p = (2.67, 5.33, and 8.00) kPa
rfi	1.50010		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
sfust	66.63	J/mol×K	269.92	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	430.00	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.79239e+01
Coeff. B	-6.30977e+03
Coeff. C	-7.23410e+01
Temperature range (K), min.	423.65
Temperature range (K), max.	572.62

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.91514e+02
Coeff. B	-1.75209e+04
Coeff. C	-2.51519e+01
Coeff. D	1.07455e-05
Temperature range (K), min.	269.15
Temperature range (K), max.	757.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Liquid-Liquid Equilibria of Formic Acid and Furfural in a Biphasic Aqueous-Organic System: Optimization of Solvent and Mixture Extractant:	https://www.doi.org/10.1021/acs.jced.8b00335
Apparatus to measure the vapor pressure of slowly decomposing compounds from 1 Pa to 105 Pa:	https://www.doi.org/10.1021/acs.jced.5b00752
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Liquid-Liquid Equilibria for the Binary Systems (Water + Di-n-butyl Phthalate), (Water + Di-ethyl Phthalate), and (Water + Di-isobutyl Hexahydrophthalate) from (298.2 to 348.2) K:	https://www.doi.org/10.1021/je050382u
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84662&Units=SI
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
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
Orrick-Erbar Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Critical Temperatures and Pressures of 12 Phthalates Using the Pulse-Heating Method:	https://www.doi.org/10.1021/je060068f
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
Vapour pressure of diethyl phthalate:	https://www.doi.org/10.1016/j.jct.2004.07.025
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1152
A Comparison of Results by Correlation Gas Chromatography with Another Gas Chromatographic Retention Time Technique. The Effects of Retention Time Coincidence on Vaporization Enthalpy and Vapor Pressure:	https://www.doi.org/10.1021/acs.jced.5b00444

(Liquid + liquid) equilibria of (water + propionic acid + diethyl phthalate) at several temperatures:	https://www.doi.org/10.1016/j.jct.2005.02.005
Solubilities of Diethyl Phthalate, Dicyclopentadiene, and Styrene in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate:	https://www.doi.org/10.1021/acs.jced.6b00901
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1152
Isobaric (vapor + liquid) equilibria of the binary system maleic anhydride and diethyl phthalate at p = (2.67, 5.33, and 8.00) kPa:	https://www.doi.org/10.1016/j.jct.2006.02.008

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
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
hfust:	Enthalpy of fusion at a given temperature
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume