Dimethyl phthalate

Other names:	1,2-BENZENEDICARBOXYLIC ACID
	1,2-Benzenedicarboxylic acid, 1,2-dimethyl ester
	1,2-Benzenedicarboxylic acid, dimethyl ester
	1,2-dimethyl phthalate
	64441-70-9
	AVOLIN
	DIMETHYL 1,2-BENZENEDICARBOXYLATE
	DIMETHYL ESTER
	DMF, Insect repellent
	DMP
	Dimethyl 1,2-benzendicarboxylate
	Dimethyl benzene-o-dicarboxylate
	Dimethyl benzeneorthodicarboxylate
	Dimethyl o-phthalate
	Dimethyl orthophthalate
	ENT 262
	Fermine
	Kemester DMP
	Kodaflex DMP
	Mipax
	NSC 15398
	NTM
	Palatinol M
	Phthalic acid, dimethyl ester
	Phthalsaeuredimethylester
	Repeftal
	Solvanom
	Solvarone
	Unimoll DM
	Uniplex 110
	dimethyl benzene-1,2-dicarboxylate
Inchi:	InChI=1S/C10H10O4/c1-13-9(11)7-5-3-4-6-8(7)10(12)14-2/h3-6H,1-2H3
InchiKey:	NIQCNGHVCWTJSM-UHFFFAOYSA-N
Formula:	C10H10O4
SMILES:	COC(=O)c1ccccc1C(=O)OC
Mol. weight [g/mol]:	194.18
CAS:	131-11-3

Physical Properties

Property code	Value	Unit	Source
chl	-4702.00	kJ/mol	NIST Webbook
chs	-4680.40 ± 2.40	kJ/mol	NIST Webbook
ea	0.55	eV	NIST Webbook
gf	-331.74	kJ/mol	Joback Method
hf	-606.10 ± 2.70	kJ/mol	NIST Webbook
hfs	-683.80 ± 2.70	kJ/mol	NIST Webbook
hfus	20.88	kJ/mol	Joback Method
hsub	77.70	kJ/mol	NIST Webbook
hvap	59.10	kJ/mol	Joback Method
ie	9.64 ± 0.07	eV	NIST Webbook
log10ws	-1.74		Aqueous Solubility Prediction Method
log10ws	-1.66		Estimated Solubility Method
logp	1.260		Crippen Method
mcvol	142.880	ml/mol	McGowan Method
pc	2770.00	kPa	Critical Temperatures and Pressures of 12 Phthalates Using the Pulse-Heating Method
rinpol	1429.44		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1454.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1425.00		NIST Webbook
rinpol	1429.29		NIST Webbook
rinpol	1431.47		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1440.94		NIST Webbook
rinpol	1441.55		NIST Webbook
rinpol	1433.14		NIST Webbook
rinpol	1431.25		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1425.00		NIST Webbook

rinpol	1416.00		NIST Webbook
rinpol	1406.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1454.00		NIST Webbook
rinpol	1460.70		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1466.20		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1406.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1481.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1406.00		NIST Webbook
rinpol	257.40		NIST Webbook
rinpol	248.00		NIST Webbook
rinpol	1437.00		NIST Webbook
rinpol	1427.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1413.00		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1417.00		NIST Webbook
ripol	2303.00		NIST Webbook
ripol	2276.00		NIST Webbook
ripol	2325.00		NIST Webbook
ripol	2303.00		NIST Webbook
sl	365.50	J/mol×K	NIST Webbook
tb	555.50	K	NIST Webbook

tb	556.80	K	(Liquid + liquid) equilibria of (water + butyric acid + esters) ternary systems
tb	557.08	K	(Liquid + liquid) equilibria of (water + propionic acid + dimethyl phthalate) at several temperatures
tb	555.20	K	NIST Webbook
tc	831.50	K	Joback Method
tf	273.20 ± 0.20	K	NIST Webbook
tf	273.00	K	NIST Webbook
tf	276.77	K	Aqueous Solubility Prediction Method
tt	274.18 ± 0.02	K	NIST Webbook
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.66	J/mol×K	831.50	Joback Method
cpg	372.43	J/mol×K	721.97	Joback Method
cpg	350.71	J/mol×K	648.95	Joback Method
cpg	338.80	J/mol×K	612.44	Joback Method
cpg	361.93	J/mol×K	685.46	Joback Method
cpg	391.31	J/mol×K	794.99	Joback Method
cpg	382.23	J/mol×K	758.48	Joback Method
cpl	303.80	J/mol×K	300.00	NIST Webbook
dvisc	0.0002254	Pa×s	574.65	Joback Method
dvisc	0.0012091	Pa×s	385.72	Joback Method
dvisc	0.0001824	Pa×s	612.44	Joback Method
dvisc	0.0005235	Pa×s	461.29	Joback Method
dvisc	0.0007664	Pa×s	423.51	Joback Method
dvisc	0.0002869	Pa×s	536.87	Joback Method
dvisc	0.0003788	Pa×s	499.08	Joback Method
hfust	16.95	kJ/mol	274.18	NIST Webbook
hfust	16.95	kJ/mol	274.20	NIST Webbook
hfust	16.95	kJ/mol	274.20	NIST Webbook
hvapt	69.40 ± 0.10	kJ/mol	365.00	NIST Webbook
hvapt	72.50 ± 0.60	kJ/mol	344.00	NIST Webbook
hvapt	74.50 ± 0.30	kJ/mol	326.00	NIST Webbook
hvapt	78.70	kJ/mol	337.50	NIST Webbook

hvapt	84.20	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	63.70	kJ/mol	459.00	NIST Webbook
hvapt	61.50	kJ/mol	492.00	NIST Webbook
hvapt	68.60	kJ/mol	408.50	NIST Webbook
rfi	1.50524		318.15	Experimental Determination and Modeling of Densities, Refractive Indices of the Binary Mixtures of Dimethylphthalate (or Dimethyladipate) + 1-Butanol, or + 2-Butanol, or + 2-Butanone at T = (288.15 to 323.15) K
rfi	1.50320		323.15	Experimental Determination and Modeling of Densities, Refractive Indices of the Binary Mixtures of Dimethylphthalate (or Dimethyladipate) + 1-Butanol, or + 2-Butanol, or + 2-Butanone at T = (288.15 to 323.15) K
rfi	1.51600		293.20	Isobaric vapor-liquid equilibria of the binary system maleic anhydride and dimethyl phthalate at 2.67, 5.33 and 8.00 kPa

rfi	1.51779	288.15	Experimental Determination and Modeling of Densities, Refractive Indices of the Binary Mixtures of Dimethylphthalate (or Dimethyladipate) + 1-Butanol, or + 2-Butanol, or + 2-Butanone at T = (288.15 to 323.15) K	
rfi	1.51565	293.15	Experimental Determination and Modeling of Densities, Refractive Indices of the Binary Mixtures of Dimethylphthalate (or Dimethyladipate) + 1-Butanol, or + 2-Butanol, or + 2-Butanone at T = (288.15 to 323.15) K	
rfi	1.51354	298.15	Experimental Determination and Modeling of Densities, Refractive Indices of the Binary Mixtures of Dimethylphthalate (or Dimethyladipate) + 1-Butanol, or + 2-Butanol, or + 2-Butanone at T = (288.15 to 323.15) K	
rfi	1.51146	303.15	Experimental Determination and Modeling of Densities, Refractive Indices of the Binary Mixtures of Dimethylphthalate (or Dimethyladipate) + 1-Butanol, or + 2-Butanol, or + 2-Butanone at T = (288.15 to 323.15) K	

rfi	1.50943		308.15	Experimental Determination and Modeling of Densities, Refractive Indices of the Binary Mixtures of Dimethylphthalate (or Dimethyladipate) + 1-Butanol, or + 2-Butanol, or + 2-Butanone at T = (288.15 to 323.15) K	
rfi	1.50736		313.15	Experimental Determination and Modeling of Densities, Refractive Indices of the Binary Mixtures of Dimethylphthalate (or Dimethyladipate) + 1-Butanol, or + 2-Butanol, or + 2-Butanone at T = (288.15 to 323.15) K	
rhol	1186.90	kg/m3	298.15	Revision of the volumetric method for measurements of liquid liquid equilibria in binary systems	
rhol	1196.23	kg/m3	288.15	Experimental Investigation of Interactions and Thermodynamic Properties of Poly(ethylene glycol) 200/400 + Dimethyl Adipate/Dimethyl Phthalate Binary Mixtures	
rhol	1163.65	kg/m3	323.15	Experimental Investigation of Interactions and Thermodynamic Properties of Poly(ethylene glycol) 200/400 + Dimethyl Adipate/Dimethyl Phthalate Binary Mixtures	

rhol	1168.28	kg/m3	318.15	Experimental Investigation of Interactions and Thermodynamic Properties of Poly(ethylene glycol) 200/400 + Dimethyl Adipate/Dimethyl Phthalate Binary Mixtures
rhol	1172.91	kg/m3	313.15	Experimental Investigation of Interactions and Thermodynamic Properties of Poly(ethylene glycol) 200/400 + Dimethyl Adipate/Dimethyl Phthalate Binary Mixtures
rhol	1182.20	kg/m3	303.15	Experimental Investigation of Interactions and Thermodynamic Properties of Poly(ethylene glycol) 200/400 + Dimethyl Adipate/Dimethyl Phthalate Binary Mixtures
rhol	1186.87	kg/m3	298.15	Experimental Investigation of Interactions and Thermodynamic Properties of Poly(ethylene glycol) 200/400 + Dimethyl Adipate/Dimethyl Phthalate Binary Mixtures
rhol	1191.54	kg/m3	293.15	Experimental Investigation of Interactions and Thermodynamic Properties of Poly(ethylene glycol) 200/400 + Dimethyl Adipate/Dimethyl Phthalate Binary Mixtures

rhol	1177.55	kg/m3	308.15	Experimental Investigation of Interactions and Thermodynamic Properties of Poly(ethylene glycol) 200/400 + Dimethyl Adipate/Dimethyl Phthalate Binary Mixtures
sfust	61.80	J/mol×K	274.18	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	389.30 ± 0.30	K	0.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.07702e+01
Coeff. B	-7.26443e+03
Coeff. C	-6.40100e+01
Temperature range (K), min.	418.67
Temperature range (K), max.	533.94

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.81743e+01
Coeff. B	-1.02413e+04
Coeff. C	-5.55726e+00
Coeff. D	-1.68650e-08
Temperature range (K), min.	272.15
Temperature range (K), max.	766.00

Sources

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 + butyric acid + esters) ternary systems:	https://www.doi.org/10.1016/j.jct.2007.01.013
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1146.mol
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Experimental Determination and Modeling of Densities, Refractive Indices of the Binary Mixtures of Dimethyl Phthalate (or Dimethyl Adipate) + 1-Butanol or + 2-Butanol, or + 2-Butanone at T = (288.15 to 323.15) K:	https://www.doi.org/10.1016/j.tca.2012.01.013
(Liquid + liquid) equilibria of (water + propionic acid + dimethyl phthalate) at T = 298.2 K:	https://www.doi.org/10.1016/j.jct.2004.12.003
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1146
Phase Equilibria for Liquid Mixtures of (an Alkane + Toluene + Dimethyl Phthalate):	https://www.doi.org/10.1021/je900592b
Revision of the volumetric method for measurements of liquid liquid equilibria in binary systems:	https://www.doi.org/10.1016/j.fluid.2004.12.004
Liquid-liquid equilibria for the aqueous mixture of C5 carboxylic acids and heavier than water solvents at T = 298.2 K:	https://www.doi.org/10.1016/j.jct.2017.12.008
Isobaric vapor-liquid equilibria of the binary system maleic anhydride and dimethyl phthalate at 2.67, 5.33 and 8.00 kPa:	https://www.doi.org/10.1016/j.fluid.2006.06.013
Liquid Phase Equilibria for Mixtures of Water + Morpholine + Ethyl Nonanoate, Dimethyl Phthalate, or Isoamyl Alcohol) at 298.15 K:	https://www.doi.org/10.1021/je1000022
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C131113&Units=SI
Experimental Investigation of Interactions and Thermodynamic Properties of Poly(ethylene glycol) 200 Phthalates Using the Pulse-Heating Technique:	https://www.doi.org/10.1021/acs.jced.5b00156
Critical Temperatures and Pressures of Phthalate Binary Mixtures:	https://www.doi.org/10.1021/je060068f
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Parametric Analysis of Mandelic Acid Separation from Aqueous Solutions by Using Secondary Amine Mixture (Amberlite LA-2) in Various Diluents:	https://www.doi.org/10.1021/acs.jced.9b00169

Legend

chl:	Standard liquid enthalpy of combustion
chs:	Standard solid 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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
rhol:	Liquid Density
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