Dibutyl phthalate

Other names:

1,2-Benzenedicarboxylic acid, 1,2-dibutyl ester
1,2-Benzenedicarboxylic acid, dibutyl ester
1,2-benzenedicarboxylic acid dibutyl ester
Benzene-o-dicarboxylic acid, di-n-butyl ester
Butyl phthalate
Celluflex DPB
DBP
DBP (ester)
DIBUTYL 1,2-BENZENEDICARBOXYLATE
Dibutyl ester of 1,2-benzenedicarboxylic acid
Dibutyl o-phthalate
Dibutyl phthalated
Dibutyl-1,2-benzenedicarboxylate
ELAOL
Ergoplast FDB
Genoplast B
Hexaplas M/B
Kodaflex DBP
Morflex 240
N-BUTYL PHTHALATE
NSC 6370
PX 104
Palatinol C
Palatinol DBP
Phthalic acid di-n-butyl ester
Phthalic acid, dibutyl ester
Polycizer DBP
RCRA waste number U069
Staflex DBP
Unimoll DB
Uniplex 150
Witcizer 300
bis-n-butyl phthalate
corflex 440
di(n-butyl) 1,2-benzenedicarboxylate
di-n-Butyl phthalate
dibutyl benzene-1,2-dicarboxylate
dibutylphthalate
hatco DBP
monocizer DBP

o-Benzenedicarboxylic acid, dibutyl ester
phthalic acid , dibutyl ester
vestinol C

Inchi: InChI=1S/C16H22O4/c1-3-5-11-19-15(17)13-9-7-8-10-14(13)16(18)20-12-6-4-2/h7-10H,3

InchiKey: DOIRQSBPFJWKBE-UHFFFAOYSA-N

Formula: C16H22O4

SMILES: CCCCOC(=O)c1ccccc1C(=O)OCCCC

Mol. weight [g/mol]: 278.34

CAS: 84-74-2

Physical Properties

Property code	Value	Unit	Source
chl	-8661.00	kJ/mol	NIST Webbook
chs	-8598.00 ± 13.00	kJ/mol	NIST Webbook
gf	-281.22	kJ/mol	Joback Method
hf	-686.30	kJ/mol	NIST Webbook
hfl	-778.00	kJ/mol	NIST Webbook
hfs	-843.00 ± 13.00	kJ/mol	NIST Webbook
hfus	36.42	kJ/mol	Joback Method
hsub	89.54	kJ/mol	NIST Webbook
hvap	91.70 ± 4.60	kJ/mol	NIST Webbook
log10ws	-4.34		Aqueous Solubility Prediction Method
log10ws	-4.40		Estimated Solubility Method
logp	3.600		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
pc	1660.00	kPa	Critical Temperatures and Pressures of 12 Phthalates Using the Pulse-Heating Method
rinpol	1963.80		NIST Webbook
rinpol	1973.00		NIST Webbook
rinpol	1909.10		NIST Webbook
rinpol	1973.86		NIST Webbook
rinpol	1976.88		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1974.00		NIST Webbook
rinpol	1909.00		NIST Webbook
rinpol	1910.00		NIST Webbook
rinpol	1910.00		NIST Webbook

rinpol	1970.00	NIST Webbook
rinpol	1913.99	NIST Webbook
rinpol	1916.64	NIST Webbook
rinpol	1917.40	NIST Webbook
rinpol	1924.51	NIST Webbook
rinpol	1930.43	NIST Webbook
rinpol	1929.33	NIST Webbook
rinpol	1921.80	NIST Webbook
rinpol	1955.00	NIST Webbook
rinpol	1965.00	NIST Webbook
rinpol	1930.00	NIST Webbook
rinpol	1915.00	NIST Webbook
rinpol	1960.00	NIST Webbook
rinpol	1960.00	NIST Webbook
rinpol	1957.00	NIST Webbook
rinpol	1957.00	NIST Webbook
rinpol	1907.00	NIST Webbook
rinpol	1972.20	NIST Webbook
rinpol	1959.00	NIST Webbook
rinpol	1936.00	NIST Webbook
rinpol	1936.00	NIST Webbook
rinpol	1937.00	NIST Webbook
rinpol	1937.00	NIST Webbook
rinpol	1937.00	NIST Webbook
rinpol	1938.00	NIST Webbook
rinpol	1947.00	NIST Webbook
rinpol	1912.00	NIST Webbook
rinpol	1923.00	NIST Webbook
rinpol	1903.00	NIST Webbook
rinpol	1909.00	NIST Webbook
rinpol	1920.00	NIST Webbook
rinpol	1923.00	NIST Webbook
rinpol	1917.00	NIST Webbook
rinpol	1966.00	NIST Webbook
rinpol	1914.00	NIST Webbook
rinpol	1961.00	NIST Webbook
rinpol	1970.00	NIST Webbook
rinpol	1954.00	NIST Webbook
rinpol	1965.00	NIST Webbook
rinpol	1922.00	NIST Webbook
rinpol	1980.00	NIST Webbook
rinpol	1970.00	NIST Webbook
rinpol	1940.00	NIST Webbook
rinpol	1973.00	NIST Webbook

rinpol	1959.00	NIST Webbook
rinpol	1970.00	NIST Webbook
rinpol	1969.00	NIST Webbook
rinpol	1925.00	NIST Webbook
rinpol	1938.00	NIST Webbook
rinpol	1940.00	NIST Webbook
rinpol	1950.00	NIST Webbook
rinpol	1930.00	NIST Webbook
rinpol	331.60	NIST Webbook
rinpol	331.60	NIST Webbook
rinpol	331.50	NIST Webbook
rinpol	324.00	NIST Webbook
rinpol	326.93	NIST Webbook
rinpol	328.00	NIST Webbook
rinpol	1915.00	NIST Webbook
rinpol	1919.00	NIST Webbook
rinpol	1959.70	NIST Webbook
rinpol	1970.00	NIST Webbook
rinpol	1967.40	NIST Webbook
rinpol	1940.00	NIST Webbook
rinpol	1924.00	NIST Webbook
rinpol	1913.00	NIST Webbook
rinpol	1922.00	NIST Webbook
rinpol	1919.00	NIST Webbook
rinpol	1926.00	NIST Webbook
rinpol	1940.00	NIST Webbook
rinpol	1938.00	NIST Webbook
rinpol	1937.00	NIST Webbook
rinpol	331.60	NIST Webbook
rinpol	1968.40	NIST Webbook
rinpol	1906.00	NIST Webbook
ripol	2680.00	NIST Webbook
ripol	2683.00	NIST Webbook
ripol	2630.00	NIST Webbook
ripol	2631.00	NIST Webbook
ripol	2618.00	NIST Webbook
ripol	2678.00	NIST Webbook
ripol	2705.00	NIST Webbook
ripol	2693.00	NIST Webbook
ripol	2680.00	NIST Webbook
ripol	2667.00	NIST Webbook
ripol	2705.00	NIST Webbook
ripol	2683.00	NIST Webbook
ripol	2680.00	NIST Webbook

ripol	2680.00		NIST Webbook
sl	561.10	J/mol×K	NIST Webbook
sl	933.00	J/mol×K	NIST Webbook
ss	514.60	J/mol×K	NIST Webbook
tb	613.20	K	(Liquid + liquid) equilibria of the (water + acetic acid + dibutyl phthalate) system
tb	608.00	K	KDB
tb	613.30	K	(Liquid + liquid) equilibria of (water + butyric acid + esters) ternary systems
tb	613.20	K	NIST Webbook
tb	613.00	K	NIST Webbook
tc	951.49	K	Joback Method
tf	238.00	K	KDB
tf	238.00	K	NIST Webbook
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.73	J/mol×K	816.98	Joback Method
cpg	663.58	J/mol×K	783.35	Joback Method
cpg	724.87	J/mol×K	951.49	Joback Method
cpg	714.48	J/mol×K	917.86	Joback Method
cpg	703.17	J/mol×K	884.24	Joback Method
cpg	690.92	J/mol×K	850.61	Joback Method
cpg	648.45	J/mol×K	749.72	Joback Method
cpl	477.00	J/mol×K	300.00	NIST Webbook
cpl	476.00	J/mol×K	298.15	NIST Webbook
cps	477.00	J/mol×K	300.00	NIST Webbook
dvisc	0.0000934	Pa×s	749.72	Joback Method
dvisc	0.0003132	Pa×s	552.13	Joback Method
dvisc	0.0002148	Pa×s	601.53	Joback Method
dvisc	0.0001560	Pa×s	650.93	Joback Method
dvisc	0.0001185	Pa×s	700.32	Joback Method
dvisc	0.0008522	Pa×s	453.34	Joback Method
dvisc	0.0004919	Pa×s	502.74	Joback Method

hvapt	84.10	kJ/mol	385.63	Synthesis and Physical and Thermodynamic Properties of Lactic Acid and Malic Acid-Based Natural Deep Eutectic Solvents
hvapt	84.00	kJ/mol	393.00	Express thermo-gravimetric method for the vaporization enthalpies appraisal for very low volatile molecular and ionic compounds.
hvapt	91.70	kJ/mol	300.50	NIST Webbook
hvapt	99.30	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	94.00	kJ/mol	391.50	NIST Webbook
hvapt	80.40	kJ/mol	462.00	NIST Webbook
hvapt	76.10	kJ/mol	536.50	NIST Webbook
rfi	1.49270		293.20	Isothermal (vapor + liquid) equilibria of maleic anhydride + di-isobutyl hexahydrophthalate and maleic anhydride + di-n-butyl phthalate systems at T= (413.2, 433.2 and 453.2) K
rhol	1047.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.71161e+01
Coeff. B	-6.41692e+03
Coeff. C	-9.08660e+01
Temperature range (K), min.	472.18
Temperature range (K), max.	634.46

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.53163e+02
Coeff. B	-2.23385e+04
Coeff. C	-3.38550e+01
Coeff. D	1.38807e-05
Temperature range (K), min.	238.15
Temperature range (K), max.	781.00

Sources

Liquid-Liquid Equilibria of Formic Acid and Furfural in a Biphasic Aqueous-Organic System: Optimization of Solvent and Amine Extractant:	https://www.doi.org/10.1021/acs.jced.8b00335
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1157.mol
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1157
A Comparison of Results by Correlation Gas Chromatography with Another Gas Chromatographic Method:	https://www.doi.org/10.1021/acs.jced.5b00444
Critical Temperatures and Pressures of 12 Phthalates Using the Pulse Heating Retention Time Technique. The Effects of Retention Time Coincidence on Vaporization Enthalpy and Vapor Pressure:	https://www.doi.org/10.1021/je060068f
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
(Liquid + liquid) equilibria of the (water + acetic acid + dibutyl phthalate) system:	https://www.doi.org/10.1016/j.jct.2005.03.003
Isothermal (vapor + liquid) equilibria of maleic anhydride + di-isobutyl hexahydrophthalate and maleic anhydride + di-n-butyl phthalate systems at T= (413.2, 433.2 and 453.2) K:	https://www.doi.org/10.1016/j.jct.2005.10.012
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84742&Units=SI
Determination of Henry's Law Constant Using Diffusion in Air and Water Boundary Layers:	https://www.doi.org/10.1021/je300954s
Express thermo-gravimetric method for the vaporization enthalpies appraisal for very low volatile molecular and ionic compounds.:	https://www.doi.org/10.1016/j.tca.2012.03.018
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
(Liquid + liquid) equilibria of (water + butyric acid + esters) ternary systems:	https://www.doi.org/10.1016/j.jct.2007.01.013
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Synthesis and Physical and Thermodynamic Properties of Lactic Acid and Malic Acid Based Natural Deep Eutectic Solvents:	https://www.doi.org/10.1021/acs.jced.7b01037
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
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

Legend

chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
cps:	Solid 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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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
nfpaf:	NFPA Fire Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sl:	Liquid phase molar entropy at standard conditions
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume