Di-n-octyl phthalate

Other names:	1,2-BENZENEDICARBOXYLIC ACID
	1,2-Benzenedicarbonic acid, dioctyl ester
	1,2-Benzenedicarboxylic acid, 1,2-dioctyl ester
	1,2-Benzenedicarboxylic acid, dioctyl ester
	Celluflex dop
	DICAPRYL PHTHALATE
	DIOCTYL ESTER
	DNOP
	Dinopol NOP
	Dioctyl 1,2-benzenedicarboxylate
	Dioctyl o-benzenedicarboxylate
	Dioctyl o-phthalate
	Dioctyl phthalate
	Dioktylester kyseliny ftalove
	N-OCTYL PHTHALATE
	NSC 15318
	Octyl phthalate
	PX-138
	Phthalic acid, dioctyl ester
	Polycizer 162
	Rcra waste number U107
	Vinicizer 85
	Vinycizer 85
	o-Benzenedicarboxylic acid, dioctyl ester
Inchi:	InChI=1S/C24H38O4/c1-3-5-7-9-11-15-19-27-23(25)21-17-13-14-18-22(21)24(26)28-20-
InchiKey:	MQIUGAXCHLFZKX-UHFFFAOYSA-N
Formula:	C24H38O4
SMILES:	CCCCCCCCOC(=O)c1ccccc1C(=O)OCCCCCCCC
Mol. weight [g/mol]:	390.56
CAS:	117-84-0

Physical Properties

Property code	Value	Unit	Source
gf	-213.86	kJ/mol	Joback Method
hf	-803.23	kJ/mol	Joback Method
hfus	57.14	kJ/mol	Joback Method

hvap	90.27	kJ/mol	Joback Method
log10ws	-5.11		Aqueous Solubility Prediction Method
log10ws	-5.12		Estimated Solubility Method
logp	6.721		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
pc	1080.00	kPa	Critical Temperatures and Pressures of 12 Phthalates Using the Pulse-Heating Method
rinpol	420.40		NIST Webbook
rinpol	2686.00		NIST Webbook
rinpol	2687.00		NIST Webbook
rinpol	2682.00		NIST Webbook
rinpol	2741.00		NIST Webbook
tb	932.76	K	Joback Method
tc	1142.45	K	Joback Method
tf	255.82	K	Aqueous Solubility Prediction Method
vc	1.319	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1179.51	J/mol×K	1072.55	Joback Method
cpg	1201.88	J/mol×K	1142.45	Joback Method
cpg	1191.30	J/mol×K	1107.50	Joback Method
cpg	1119.44	J/mol×K	932.76	Joback Method
cpg	1136.46	J/mol×K	967.71	Joback Method
cpg	1152.13	J/mol×K	1002.66	Joback Method
cpg	1166.46	J/mol×K	1037.60	Joback Method
dvisc	0.0000544	Pa×s	803.01	Joback Method
dvisc	0.0000401	Pa×s	867.88	Joback Method
dvisc	0.0000308	Pa×s	932.76	Joback Method
dvisc	0.0003848	Pa×s	543.50	Joback Method
dvisc	0.0002018	Pa×s	608.38	Joback Method
dvisc	0.0001199	Pa×s	673.25	Joback Method
dvisc	0.0000780	Pa×s	738.13	Joback Method

hvapt	122.70	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	
rfi	1.48100		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	1.48310		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	1.48500		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	

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.29723e+01
Coeff. B	-4.89620e+03
Coeff. C	-1.22804e+02
Temperature range (K), min.	508.80
Temperature range (K), max.	761.92

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.27880e+01
Coeff. B	-1.19674e+04
Coeff. C	1.07854e-04
Coeff. D	-9.54457e-11
Temperature range (K), min.	423.15
Temperature range (K), max.	523.15

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C117840&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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 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
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
Crippen 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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1161.mol
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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=1161

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	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
nfpaf:	NFPA Fire Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume