1,2-Benzenedicarboxylic acid, dipropyl ester

Other names:	1,2-benzenedicarboxylic acid dipropyl ester
	DI-N-PROPYL PHTHALATE
	Dipropyl phthalate
	Phthalic acid di-n-propyl ester
	Phthalic acid, dipropyl ester
	dipropyl benzene-1,2-dicarboxylate
Inchi:	InChI=1S/C14H18O4/c1-3-9-17-13(15)11-7-5-6-8-12(11)14(16)18-10-4-2/h5-8H,3-4,9-10
InchiKey:	MQHNKCZKNAJROC-UHFFFAOYSA-N
Formula:	C14H18O4
SMILES:	CCCOC(=O)c1ccccc1C(=O)OCCC
Mol. weight [g/mol]:	250.29
CAS:	131-16-8

Physical Properties

Property code	Value	Unit	Source
gf	-298.06	kJ/mol	Joback Method
hf	-596.83	kJ/mol	Joback Method
hfus	31.24	kJ/mol	Joback Method
hvap	68.01	kJ/mol	Joback Method
log10ws	-3.82		Aqueous Solubility Prediction Method
logp	2.820		Crippen Method
mcvol	199.240	ml/mol	McGowan Method
pc	1900.00	kPa	Critical Temperatures and Pressures of 12 Phthalates Using the Pulse-Heating Method
rinpol	1735.23		NIST Webbook
rinpol	1743.56		NIST Webbook
rinpol	1745.58		NIST Webbook
rinpol	1742.96		NIST Webbook
rinpol	1735.96		NIST Webbook
rinpol	1735.27		NIST Webbook
rinpol	1746.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1742.96		NIST Webbook
rinpol	1743.00		NIST Webbook
rinpol	1756.00		NIST Webbook

rinpol	1733.62		NIST Webbook
rinpol	1756.00		NIST Webbook
rinpol	1743.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1760.00		NIST Webbook
rinpol	1735.27		NIST Webbook
tb	577.70	K	NIST Webbook
tb	590.70	K	NIST Webbook
tc	909.90	K	Joback Method
tf	430.80	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.98	J/mol×K	703.96	Joback Method
cpg	554.36	J/mol×K	738.28	Joback Method
cpg	567.84	J/mol×K	772.61	Joback Method
cpg	580.44	J/mol×K	806.93	Joback Method
cpg	592.16	J/mol×K	841.25	Joback Method
cpg	603.00	J/mol×K	875.58	Joback Method
cpg	612.97	J/mol×K	909.90	Joback Method
dvisc	0.0009874	Pa×s	430.80	Joback Method
dvisc	0.0005866	Pa×s	476.33	Joback Method
dvisc	0.0003816	Pa×s	521.85	Joback Method
dvisc	0.0002660	Pa×s	567.38	Joback Method
dvisc	0.0001956	Pa×s	612.91	Joback Method
dvisc	0.0001501	Pa×s	658.43	Joback Method
dvisc	0.0001192	Pa×s	703.96	Joback Method
hvapt	73.20	kJ/mol	490.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	442.00 ± 1.00	K	0.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.98607e+01
Coeff. B	-8.80513e+03
Coeff. C	-1.38970e-04
Coeff. D	1.22195e-10
Temperature range (K), min.	403.15
Temperature range (K), max.	523.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C131168&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1156
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1156.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
pc:	Critical Pressure

pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume