1,2-Benzenedicarboxylic acid, dihexyl ester

Other names:	Dihexyl phthalate
	Dihexylester kyseliny ftalove
	Phthalic acid, dihexyl ester
	di-n-Hexyl phthalate
	dihexyl benzene-1,2-dicarboxylate
Inchi:	InChI=1S/C20H30O4/c1-3-5-7-11-15-23-19(21)17-13-9-10-14-18(17)20(22)24-16-12-8-6
InchiKey:	KCXZNSGUUQJJTR-UHFFFAOYSA-N
Formula:	C20H30O4
SMILES:	CCCCCCOC(=O)c1ccccc1C(=O)OCCCCCC
Mol. weight [g/mol]:	334.45
CAS:	84-75-3

Physical Properties

Property code	Value	Unit	Source
gf	-247.54	kJ/mol	Joback Method
hf	-720.67	kJ/mol	Joback Method
hfus	46.78	kJ/mol	Joback Method
hvap	81.36	kJ/mol	Joback Method
log10ws	-5.94		Aqueous Solubility Prediction Method
log10ws	-6.14		Estimated Solubility Method
logp	5.161		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1340.00	kPa	Critical Temperatures and Pressures of 12 Phthalates Using the Pulse-Heating Method
rinpol	2281.00		NIST Webbook
rinpol	2305.00		NIST Webbook
rinpol	2308.00		NIST Webbook
tb	841.24	K	Joback Method
tc	1041.25	K	Joback Method
tf	498.42	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.72	J/mol×K	841.24	Joback Method
cpg	893.85	J/mol×K	874.57	Joback Method
cpg	908.85	J/mol×K	907.91	Joback Method
cpg	922.75	J/mol×K	941.24	Joback Method
cpg	935.56	J/mol×K	974.58	Joback Method
cpg	947.32	J/mol×K	1007.91	Joback Method
cpg	958.03	J/mol×K	1041.25	Joback Method
dvisc	0.0005930	Pa×s	498.42	Joback Method
dvisc	0.0003251	Pa×s	555.56	Joback Method
dvisc	0.0001994	Pa×s	612.69	Joback Method
dvisc	0.0001329	Pa×s	669.83	Joback Method
dvisc	0.0000945	Pa×s	726.97	Joback Method
dvisc	0.0000705	Pa×s	784.10	Joback Method
dvisc	0.0000548	Pa×s	841.24	Joback Method

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C84753&Units=SI

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

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

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume