Dihexyl phthalate

Other names:	1,2-benzenedicarboxylic acid, dihexyl ester
	Dihexylester kyseliny ftalove
	di-n-Hexyl phthalate
	dihexyl benzene-1,2-dicarboxylate
	phthalic acid, dihexyl ester
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]:	334.46

Physical Properties

Property code	Value	Unit	Source
af	1.0110		Cheméo Relay (1.0)
hf	-819.92	kJ/mol	Cheméo Relay (1.0)
hfus	46.78	kJ/mol	Joback Method
hvap	94.73	kJ/mol	Cheméo Relay (1.0)
ie	9.15	eV	Cheméo Relay (1.0)
log10ws	-6.14		Estimated Solubility Method
log10ws	-5.94		Aqueous Solubility Prediction 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	2308.00		NIST Webbook
rinpol	2308.00		NIST Webbook
rinpol	2305.00		NIST Webbook
rinpol	2281.00		NIST Webbook
rinpol	2308.00		NIST Webbook
rinpol	2305.00		NIST Webbook
rinpol	2306.00		NIST Webbook
rinpol	2306.00		NIST Webbook
rinpol	2331.00		NIST Webbook
rinpol	2281.00		NIST Webbook
rinpol	2272.00		NIST Webbook

tb	631.70	K	Cheméo Relay (1.0)
tc	832.30	K	Cheméo Relay (1.0)
tf	259.87	K	Cheméo Relay (1.0)
vc	1.073	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	958.03	J/mol×K	1041.25	Joback Method
cpg	935.56	J/mol×K	974.58	Joback Method
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	947.32	J/mol×K	1007.91	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
hvapt	92.00	kJ/mol	493.00	NIST Webbook
hvapt	103.00	kJ/mol	365.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	459.50 ± 1.50	K	0.07	NIST Webbook

Sources

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

Cheméo Relay (1.0):

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
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Cheméo Relay (1.0, beta):	
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84753&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume