Diamyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, 1,2-dipentyl ester
	1,2-Benzenedicarboxylic acid, dipentyl ester
	1,2-benzenedicarboxylic acid dipentyl ester
	1,2-benzenedioic acid, dipentyl ester
	Amoil
	Amyl phthalate
	Di-n-pentyl phthalate
	Dipentyl phthalate
	NSC 4720
	Phthalic acid, dipentyl ester
	di-n-Amyl phthalate
	di-n-pentyl o-phthalate
	dipentyl 1,2-butanedioate
	dipentyl benzene-1,2-dicarboxylate
	phthalic acid dipentyl ester
Inchi:	InChI=1S/C18H26O4/c1-3-5-9-13-21-17(19)15-11-7-8-12-16(15)18(20)22-14-10-6-4-2/h7
InchiKey:	IPKKHRVROFYTEK-UHFFFAOYSA-N
Formula:	C18H26O4
SMILES:	CCCCCOC(=O)c1ccccc1C(=O)OCCCCC
Mol. weight [g/mol]:	306.40
CAS:	131-18-0

Physical Properties

Property code	Value	Unit	Source
chs	-9875.00 ± 13.00	kJ/mol	NIST Webbook
gf	-264.38	kJ/mol	Joback Method
hf	-679.39	kJ/mol	Joback Method
hfs	-924.00 ± 13.00	kJ/mol	NIST Webbook
hfus	41.60	kJ/mol	Joback Method
hvap	76.91	kJ/mol	Joback Method
log10ws	-3.49		Aqueous Solubility Prediction Method
logp	4.381		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1430.00	kPa	Critical Temperatures and Pressures of 12 Phthalates Using the Pulse-Heating Method

rinpol	2120.00		NIST Webbook
rinpol	2127.00		NIST Webbook
rinpol	2140.00		NIST Webbook
rinpol	2136.00		NIST Webbook
rinpol	2140.00		NIST Webbook
rinpol	2122.00		NIST Webbook
rinpol	2120.00		NIST Webbook
rinpol	2121.00		NIST Webbook
tb	795.48	K	Joback Method
tc	995.15	K	Joback Method
tf	475.88	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	817.75	J/mol×K	928.59	Joback Method
cpg	839.97	J/mol×K	995.15	Joback Method
cpg	829.35	J/mol×K	961.87	Joback Method
cpg	761.25	J/mol×K	795.48	Joback Method
cpg	776.92	J/mol×K	828.76	Joback Method
cpg	791.55	J/mol×K	862.04	Joback Method
cpg	805.16	J/mol×K	895.32	Joback Method
dvisc	0.0000720	Pa×s	795.48	Joback Method
dvisc	0.0001223	Pa×s	688.95	Joback Method
dvisc	0.0000921	Pa×s	742.21	Joback Method
dvisc	0.0007181	Pa×s	475.88	Joback Method
dvisc	0.0004036	Pa×s	529.15	Joback Method
dvisc	0.0002520	Pa×s	582.41	Joback Method
dvisc	0.0001703	Pa×s	635.68	Joback Method
hvapt	99.20	kJ/mol	373.00	NIST Webbook
hvapt	87.30	kJ/mol	356.50	NIST Webbook
hvapt	99.40	kJ/mol	401.50	NIST Webbook

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C131180&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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume