Dibenzyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, bis(phenylmethyl) ester
	Phthalic acid, dibenzyl ester
	Benzyl phthalate
	Dibenzyl ester of 1,2-benzenedicarboxylic acid
Inchi:	InChI=1S/C22H18O4/c23-21(25-15-17-9-3-1-4-10-17)19-13-7-8-14-20(19)22(24)26-16-1
InchiKey:	UCVPKAZCQPRWAY-UHFFFAOYSA-N
Formula:	C22H18O4
SMILES:	O=C(OCc1ccccc1)c1ccccc1C(=O)OCc1ccccc1
Mol. weight [g/mol]:	346.38
CAS:	523-31-9

Physical Properties

Property code	Value	Unit	Source
gf	-5.88	kJ/mol	Joback Method
hf	-288.89	kJ/mol	Joback Method
hfus	40.04	kJ/mol	Joback Method
hvap	90.37	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	4.401		Crippen Method
mcvol	264.440	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinpol	2690.00		NIST Webbook
tb	940.36	K	Joback Method
tc	1190.02	K	Joback Method
tf	573.80	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.82	J/mol×K	940.36	Joback Method
cpg	840.50	J/mol×K	1148.41	Joback Method
cpg	833.81	J/mol×K	1106.80	Joback Method
cpg	825.88	J/mol×K	1065.19	Joback Method

cpg	816.62	J/mol×K	1023.58	Joback Method
cpg	805.96	J/mol×K	981.97	Joback Method
cpg	846.02	J/mol×K	1190.02	Joback Method
dvisc	0.0000438	Pa×s	940.36	Joback Method
dvisc	0.0000553	Pa×s	879.27	Joback Method
dvisc	0.0000724	Pa×s	818.17	Joback Method
dvisc	0.0000990	Pa×s	757.08	Joback Method
dvisc	0.0001429	Pa×s	695.99	Joback Method
dvisc	0.0002214	Pa×s	634.89	Joback Method
dvisc	0.0003766	Pa×s	573.80	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C523319&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

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