

Phthalic acid, 2,4-dichlorobenzyl pentadecyl ester

Inchi:	InChI=1S/C30H40Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-21-35-29(33)26-17-14-15-18
InchiKey:	OQJCEWMAXFVYIG-UHFFFAOYSA-N
Formula:	C30H40Cl2O4
SMILES:	CCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	535.54

Physical Properties

Property code	Value	Unit	Source
gf	-94.05	kJ/mol	Joback Method
hf	-744.96	kJ/mol	Joback Method
hfus	74.34	kJ/mol	Joback Method
hvap	115.99	kJ/mol	Joback Method
log10ws	-11.30		Crippen Method
logp	9.598		Crippen Method
mvol	425.400	ml/mol	McGowan Method
pc	833.86	kPa	Joback Method
rinpol	3693.00		NIST Webbook
tb	1181.54	K	Joback Method
tc	1456.46	K	Joback Method
tf	722.42	K	Joback Method
vc	1.645	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1421.42	J/molxK	1181.54	Joback Method
cpg	1462.54	J/molxK	1410.64	Joback Method
cpg	1457.76	J/molxK	1364.82	Joback Method
cpg	1451.38	J/molxK	1319.00	Joback Method
cpg	1443.28	J/molxK	1273.18	Joback Method
cpg	1433.33	J/molxK	1227.36	Joback Method
cpg	1465.84	J/molxK	1456.46	Joback Method
dvisc	0.0000093	Paxs	1181.54	Joback Method
dvisc	0.0000119	Paxs	1105.02	Joback Method

dvisc	0.0000157	Paxs	1028.50	Joback Method
dvisc	0.0000216	Paxs	951.98	Joback Method
dvisc	0.0000316	Paxs	875.46	Joback Method
dvisc	0.0000497	Paxs	798.94	Joback Method
dvisc	0.0000858	Paxs	722.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382569&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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