Phthalic acid, di(4-chloro-2-methoxybenzyl) ester

Inchi: InChI=1S/C24H20Cl2O6/c1-29-21-11-17(25)9-7-15(21)13-31-23(27)19-5-3-4-6-20(19)24

InchiKey: LDIUBONKJQBVDK-UHFFFAOYSA-N

Formula: C24H20Cl2O6

SMILES: COc1cc(Cl)ccc1COC(=O)c1ccccc1C(=O)OCc1ccc(Cl)cc1OC

Mol. weight [g/mol]: 475.32

Physical Properties

Property code	Value	Unit	Source
gf	-261.42	kJ/mol	Joback Method
hf	-671.97	kJ/mol	Joback Method
hfus	54.44	kJ/mol	Joback Method
hvap	111.06	kJ/mol	Joback Method
log10ws	-7.79		Crippen Method
logp	5.725		Crippen Method
mcvol	328.840	ml/mol	McGowan Method
pc	1456.79	kPa	Joback Method
rinpol	3457.00		NIST Webbook
rinpol	3457.00		NIST Webbook
tb	1125.74	K	Joback Method
tc	1383.51	K	Joback Method
tf	750.72	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.96	J/mol×K	1125.74	Joback Method
cpg	985.55	J/mol×K	1168.70	Joback Method
cpg	988.02	J/mol×K	1211.66	Joback Method
cpg	988.37	J/mol×K	1254.63	Joback Method
cpg	986.60	J/mol×K	1297.59	Joback Method
cpg	982.73	J/mol×K	1340.55	Joback Method
cpg	976.74	J/mol×K	1383.51	Joback Method
dvisc	0.0000755	Pa×s	750.72	Joback Method

dvisc	0.0000515	Pa×s	813.22	Joback Method
dvisc	0.0000371	Pa×s	875.73	Joback Method
dvisc	0.0000279	Pa×s	938.23	Joback Method
dvisc	0.0000218	Pa×s	1000.73	Joback Method
dvisc	0.0000175	Pa×s	1063.24	Joback Method
dvisc	0.0000144	Pa×s	1125.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382847&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

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