

Isophthalic acid, di(2-chloro-5-methylphenyl) ester

Inchi:	InChI=1S/C22H16Cl2O4/c1-13-6-8-17(23)19(10-13)27-21(25)15-4-3-5-16(12-15)22(26)2
InchiKey:	TWTRJLJIQDYMBM-UHFFFAOYSA-N
Formula:	C22H16Cl2O4
SMILES:	Cc1ccc(Cl)c(OC(=O)c2cccc(C(=O)Oc3cc(C)ccc3Cl)c2)c1
Mol. weight [g/mol]:	415.27

Physical Properties

Property code	Value	Unit	Source
gf	-68.26	kJ/mol	Joback Method
hf	-366.25	kJ/mol	Joback Method
hfus	46.88	kJ/mol	Joback Method
hvap	101.79	kJ/mol	Joback Method
log10ws	-7.97		Crippen Method
logp	6.049		Crippen Method
mvol	288.920	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpol	3420.00		NIST Webbook
rinpol	3420.00		NIST Webbook
tb	1035.14	K	Joback Method
tc	1292.95	K	Joback Method
tf	683.72	K	Joback Method
vc	1.089	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.17	J/molxK	1035.14	Joback Method
cpg	831.58	J/molxK	1078.11	Joback Method
cpg	838.47	J/molxK	1121.08	Joback Method
cpg	843.89	J/molxK	1164.05	Joback Method
cpg	847.87	J/molxK	1207.02	Joback Method
cpg	850.45	J/molxK	1249.98	Joback Method
cpg	851.70	J/molxK	1292.95	Joback Method
dvisc	0.0001839	Paxs	683.72	Joback Method

dvisc	0.0001256	Paxs	742.29	Joback Method
dvisc	0.0000907	Paxs	800.86	Joback Method
dvisc	0.0000685	Paxs	859.43	Joback Method
dvisc	0.0000536	Paxs	918.00	Joback Method
dvisc	0.0000432	Paxs	976.57	Joback Method
dvisc	0.0000356	Paxs	1035.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356573&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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