Isophthalic acid, di(4-chloro-3-methylphenyl) ester

Inchi: InChI=1S/C22H16Cl2O4/c1-13-10-17(6-8-19(13)23)27-21(25)15-4-3-5-16(12-15)22(26)2
InchiKey: SUSUOKMPOCEJFE-UHFFFAOYSA-N
Formula: C22H16Cl2O4
SMILES: Cc1cc(OC(=O)c2cccc(C(=O)Oc3ccc(Cl)c(C)c3)c2)ccc1Cl
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
mcvol	288.920	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpol	3535.00		NIST Webbook
rinpol	3535.00		NIST Webbook
tb	1035.14	K	Joback Method
tc	1292.95	K	Joback Method
tf	683.72	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001256	Pa×s	742.29	Joback Method
dvisc	0.0000907	Pa×s	800.86	Joback Method
dvisc	0.0000685	Pa×s	859.43	Joback Method
dvisc	0.0000536	Pa×s	918.00	Joback Method
dvisc	0.0000432	Pa×s	976.57	Joback Method
dvisc	0.0000356	Pa×s	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=U344598&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