Isophthalic acid, di(3-chlorophenyl) ester

Inchi: InChI=1S/C20H12Cl2O4/c21-15-6-2-8-17(11-15)25-19(23)13-4-1-5-14(10-13)20(24)26-1
InchiKey: JODVTEUNZDZENC-UHFFFAOYSA-N
Formula: C20H12Cl2O4
SMILES: O=C(Oc1cccc(Cl)c1)c1cccc(C(=O)Oc2cccc(Cl)c2)c1
Mol. weight [g/mol]: 387.21

Physical Properties

Property code	Value	Unit	Source
gf	-65.84	kJ/mol	Joback Method
hf	-302.03	kJ/mol	Joback Method
hfus	42.48	kJ/mol	Joback Method
hvap	96.01	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	5.432		Crippen Method
mcvol	260.740	ml/mol	McGowan Method
pc	2119.73	kPa	Joback Method
rinpol	3273.00		NIST Webbook
rinpol	3273.00		NIST Webbook
tb	979.42	K	Joback Method
tc	1241.84	K	Joback Method
tf	636.14	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.74	J/mol×K	979.42	Joback Method
cpg	722.47	J/mol×K	1023.16	Joback Method
cpg	729.76	J/mol×K	1066.89	Joback Method
cpg	735.69	J/mol×K	1110.63	Joback Method
cpg	740.32	J/mol×K	1154.37	Joback Method
cpg	743.69	J/mol×K	1198.11	Joback Method
cpg	745.87	J/mol×K	1241.84	Joback Method
dvisc	0.0002654	Pa×s	636.14	Joback Method

dvisc	0.0001748	Pa×s	693.35	Joback Method
dvisc	0.0001227	Pa×s	750.57	Joback Method
dvisc	0.0000905	Pa×s	807.78	Joback Method
dvisc	0.0000696	Pa×s	864.99	Joback Method
dvisc	0.0000552	Pa×s	922.21	Joback Method
dvisc	0.0000450	Pa×s	979.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344609&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