Isophthalic acid, di(2,6-dichlorophenyl) ester

Inchi: InChI=1S/C20H10Cl4O4/c21-13-6-2-7-14(22)17(13)27-19(25)11-4-1-5-12(10-11)20(26)2
InchiKey: IHVFCYRCZIWGCQ-UHFFFAOYSA-N
Formula: C20H10Cl4O4
SMILES: O=C(Oc1c(Cl)cccc1Cl)c1cccc(C(=O)Oc2c(Cl)cccc2Cl)c1
Mol. weight [g/mol]: 456.10

Physical Properties

Property code	Value	Unit	Source
gf	-108.96	kJ/mol	Joback Method
hf	-356.45	kJ/mol	Joback Method
hfus	50.10	kJ/mol	Joback Method
hvap	106.10	kJ/mol	Joback Method
log10ws	-8.39		Crippen Method
logp	6.739		Crippen Method
mcvol	285.220	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rinpol	3489.00		NIST Webbook
rinpol	3489.00		NIST Webbook
tb	1064.24	K	Joback Method
tc	1332.44	K	Joback Method
tf	721.02	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.89	J/mol×K	1064.24	Joback Method
cpg	752.38	J/mol×K	1287.74	Joback Method
cpg	752.34	J/mol×K	1243.04	Joback Method
cpg	751.01	J/mol×K	1198.34	Joback Method
cpg	748.36	J/mol×K	1153.64	Joback Method
cpg	744.33	J/mol×K	1108.94	Joback Method
cpg	751.20	J/mol×K	1332.44	Joback Method
dvisc	0.0000343	Pa×s	1064.24	Joback Method

dvisc	0.0000412	Pa×s	1007.04	Joback Method
dvisc	0.0000507	Pa×s	949.83	Joback Method
dvisc	0.0000641	Pa×s	892.63	Joback Method
dvisc	0.0000835	Pa×s	835.43	Joback Method
dvisc	0.0001132	Pa×s	778.22	Joback Method
dvisc	0.0001611	Pa×s	721.02	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344629&Units=SI

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