Isophthalic acid, isohexyl pentachlorophenyl ester

Inchi: InChI=1S/C20H17Cl5O4/c1-10(2)5-4-8-28-19(26)11-6-3-7-12(9-11)20(27)29-18-16(24)14
InchiKey: VNSVEQGJUAHDPB-UHFFFAOYSA-N
Formula: C20H17Cl5O4
SMILES: CC(C)CCCOC(=O)c1cccc(C(=O)Oc2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl)c1
Mol. weight [g/mol]: 498.61

Physical Properties

Property code	Value	Unit	Source
gf	-245.37	kJ/mol	Joback Method
hf	-625.47	kJ/mol	Joback Method
hfus	56.34	kJ/mol	Joback Method
hvap	108.49	kJ/mol	Joback Method
log10ws	-9.08		Crippen Method
logp	7.766		Crippen Method
mcvol	321.220	ml/mol	McGowan Method
pc	1422.92	kPa	Joback Method
rinpol	3380.00		NIST Webbook
rinpol	3380.00		NIST Webbook
tb	1079.53	K	Joback Method
tc	1330.07	K	Joback Method
tf	722.04	K	Joback Method
vc	1.226	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	869.29	J/mol×K	1079.53	Joback Method
cpg	887.49	J/mol×K	1288.31	Joback Method
cpg	886.68	J/mol×K	1246.55	Joback Method
cpg	884.48	J/mol×K	1204.80	Joback Method
cpg	880.87	J/mol×K	1163.04	Joback Method
cpg	875.81	J/mol×K	1121.29	Joback Method
cpg	886.91	J/mol×K	1330.07	Joback Method
dvisc	0.0000256	Pa×s	1079.53	Joback Method

dvisc	0.0000311	Pa×s	1019.95	Joback Method
dvisc	0.0000387	Pa×s	960.37	Joback Method
dvisc	0.0000495	Pa×s	900.78	Joback Method
dvisc	0.0000656	Pa×s	841.20	Joback Method
dvisc	0.0000908	Pa×s	781.62	Joback Method
dvisc	0.0001325	Pa×s	722.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356578&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