Isophthalic acid, hexyl pentachlorophenyl ester

Inchi: InChI=1S/C20H17Cl5O4/c1-2-3-4-5-9-28-19(26)11-7-6-8-12(10-11)20(27)29-18-16(24)14

InchiKey: REKFDACZCXFMAM-UHFFFAOYSA-N

Formula: C20H17Cl5O4

SMILES: CCCCCCOC(=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	-242.93	kJ/mol	Joback Method
hf	-620.19	kJ/mol	Joback Method
hfus	59.86	kJ/mol	Joback Method
hvap	108.87	kJ/mol	Joback Method
log10ws	-9.32		Crippen Method
logp	7.910		Crippen Method
mcvol	321.220	ml/mol	McGowan Method
pc	1414.37	kPa	Joback Method
rinpol	3423.00		NIST Webbook
rinpol	3423.00		NIST Webbook
tb	1079.97	K	Joback Method
tc	1328.98	K	Joback Method
tf	737.04	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	869.02	J/mol×K	1079.97	Joback Method
cpg	875.61	J/mol×K	1121.47	Joback Method
cpg	880.77	J/mol×K	1162.97	Joback Method
cpg	884.53	J/mol×K	1204.47	Joback Method
cpg	886.90	J/mol×K	1245.97	Joback Method
cpg	887.92	J/mol×K	1287.48	Joback Method
cpg	887.58	J/mol×K	1328.98	Joback Method
dvisc	0.0001301	Pa×s	737.04	Joback Method

dvisc	0.0000921	Pa×s	794.19	Joback Method
dvisc	0.0000682	Pa×s	851.35	Joback Method
dvisc	0.0000525	Pa×s	908.50	Joback Method
dvisc	0.0000417	Pa×s	965.66	Joback Method
dvisc	0.0000339	Pa×s	1022.82	Joback Method
dvisc	0.0000282	Pa×s	1079.97	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U356579&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