Isophthalic acid, pentachlorophenyl pentyl ester

Inchi: InChI=1S/C19H15Cl5O4/c1-2-3-4-8-27-18(25)10-6-5-7-11(9-10)19(26)28-17-15(23)13(21
InchiKey: HLZIMBQKVPWIMC-UHFFFAOYSA-N
Formula: C19H15Cl5O4
SMILES: CCCCCOC(=O)c1cccc(C(=O)Oc2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl)c1
Mol. weight [g/mol]: 484.58

Physical Properties

Property code	Value	Unit	Source
gf	-251.35	kJ/mol	Joback Method
hf	-599.55	kJ/mol	Joback Method
hfus	57.27	kJ/mol	Joback Method
hvap	106.65	kJ/mol	Joback Method
log10ws	-8.90		Crippen Method
logp	7.520		Crippen Method
mcvol	307.130	ml/mol	McGowan Method
pc	1522.31	kPa	Joback Method
rinpol	3320.00		NIST Webbook
rinpol	3320.00		NIST Webbook
tb	1057.09	K	Joback Method
tc	1305.32	K	Joback Method
tf	725.77	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	811.99	J/mol×K	1057.09	Joback Method
cpg	831.22	J/mol×K	1263.95	Joback Method
cpg	830.06	J/mol×K	1222.57	Joback Method
cpg	827.58	J/mol×K	1181.20	Joback Method
cpg	823.75	J/mol×K	1139.83	Joback Method
cpg	818.56	J/mol×K	1098.46	Joback Method
cpg	831.06	J/mol×K	1305.32	Joback Method
dvisc	0.0000329	Pa×s	1057.09	Joback Method

dvisc	0.0000394	Pa×s	1001.87	Joback Method
dvisc	0.0000481	Pa×s	946.65	Joback Method
dvisc	0.0000603	Pa×s	891.43	Joback Method
dvisc	0.0000779	Pa×s	836.21	Joback Method
dvisc	0.0001043	Pa×s	780.99	Joback Method
dvisc	0.0001461	Pa×s	725.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356577&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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