Isophthalic acid, isobutyl pentachlorophenyl ester

Inchi: InChI=1S/C18H13Cl5O4/c1-8(2)7-26-17(24)9-4-3-5-10(6-9)18(25)27-16-14(22)12(20)11(

InchiKey: LSEIWOOCOOPTAH-UHFFFAOYSA-N

Formula: C18H13Cl5O4

SMILES: CC(C)COC(=O)c1cccc(C(=O)Oc2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl)c1

Mol. weight [g/mol]: 470.56

Physical Properties

Property code	Value	Unit	Source
gf	-262.21	kJ/mol	Joback Method
hf	-584.19	kJ/mol	Joback Method
hfus	51.16	kJ/mol	Joback Method
hvap	104.04	kJ/mol	Joback Method
log10ws	-8.24		Crippen Method
logp	6.986		Crippen Method
mcvol	293.040	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
rinpol	3167.00		NIST Webbook
rinpol	3167.00		NIST Webbook
tb	1033.77	K	Joback Method
tc	1284.55	K	Joback Method
tf	699.50	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.84	J/mol×K	1033.77	Joback Method
cpg	762.31	J/mol×K	1075.57	Joback Method
cpg	767.41	J/mol×K	1117.36	Joback Method
cpg	771.15	J/mol×K	1159.16	Joback Method
cpg	773.54	J/mol×K	1200.96	Joback Method
cpg	774.59	J/mol×K	1242.75	Joback Method
cpg	774.31	J/mol×K	1284.55	Joback Method
dvisc	0.0001670	Pa×s	699.50	Joback Method

dvisc	0.0001167	Pa×s	755.21	Joback Method
dvisc	0.0000857	Pa×s	810.92	Joback Method
dvisc	0.0000655	Pa×s	866.63	Joback Method
dvisc	0.0000517	Pa×s	922.35	Joback Method
dvisc	0.0000419	Pa×s	978.06	Joback Method
dvisc	0.0000347	Pa×s	1033.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356575&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