Isophthalic acid, butyl pentachlorophenyl ester

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

InchiKey: YHXRPAPWRHPVTM-UHFFFAOYSA-N

Formula: C18H13Cl5O4

SMILES: CCCCOC(=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	-259.77	kJ/mol	Joback Method
hf	-578.91	kJ/mol	Joback Method
hfus	54.68	kJ/mol	Joback Method
hvap	104.42	kJ/mol	Joback Method
log10ws	-8.48		Crippen Method
logp	7.130		Crippen Method
mcvol	293.040	ml/mol	McGowan Method
pc	1643.09	kPa	Joback Method
rinpol	3220.00		NIST Webbook
tb	1034.21	K	Joback Method
tc	1282.63	K	Joback Method
tf	714.50	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.45	J/mol×K	1034.21	Joback Method
cpg	774.80	J/mol×K	1241.23	Joback Method
cpg	773.55	J/mol×K	1199.82	Joback Method
cpg	771.00	J/mol×K	1158.42	Joback Method
cpg	767.14	J/mol×K	1117.02	Joback Method
cpg	761.96	J/mol×K	1075.61	Joback Method
cpg	774.76	J/mol×K	1282.63	Joback Method
dvisc	0.0000382	Pa×s	1034.21	Joback Method
dvisc	0.0000456	Pa×s	980.92	Joback Method

dvisc	0.0000555	Pa×s	927.64	Joback Method
dvisc	0.0000692	Pa×s	874.36	Joback Method
dvisc	0.0000888	Pa×s	821.07	Joback Method
dvisc	0.0001180	Pa×s	767.78	Joback Method
dvisc	0.0001635	Pa×s	714.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356576&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