Phthalic acid, isobutyl pentafluorophenyl ester

Inchi: InChI=1S/C18H13F5O4/c1-8(2)7-26-17(24)9-5-3-4-6-10(9)18(25)27-16-14(22)12(20)11(
InchiKey: UJMANWUXNOAHJG-UHFFFAOYSA-N
Formula: C18H13F5O4
SMILES: CC(C)COC(=O)c1ccccc1C(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 388.29

Physical Properties

Property code	Value	Unit	Source
gf	-1176.61	kJ/mol	Joback Method
hf	-1486.04	kJ/mol	Joback Method
hfus	45.57	kJ/mol	Joback Method
hvap	78.03	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	4.414		Crippen Method
mcvol	240.690	ml/mol	McGowan Method
pc	1601.28	kPa	Joback Method
rinpol	2022.00		NIST Webbook
rinpol	2022.00		NIST Webbook
tb	842.97	K	Joback Method
tc	1046.62	K	Joback Method
tf	552.85	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.72	J/mol×K	842.97	Joback Method
cpg	711.00	J/mol×K	876.91	Joback Method
cpg	721.29	J/mol×K	910.85	Joback Method
cpg	730.59	J/mol×K	944.79	Joback Method
cpg	738.90	J/mol×K	978.74	Joback Method
cpg	746.22	J/mol×K	1012.68	Joback Method
cpg	752.56	J/mol×K	1046.62	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356190&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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