2,6-Di-isopropylphenol, pentafluorobenzoyl ester

Inchi: InChI=1S/C19H17F5O2/c1-8(2)10-6-5-7-11(9(3)4)18(10)26-19(25)12-13(20)15(22)17(24
InchiKey: FTZUOFGNLYCADL-UHFFFAOYSA-N
Formula: C19H17F5O2
SMILES: CC(C)c1cccc(C(C)C)c1OC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 372.33

Physical Properties

Property code	Value	Unit	Source
gf	-946.34	kJ/mol	Joback Method
hf	-1278.63	kJ/mol	Joback Method
hfus	41.47	kJ/mol	Joback Method
hvap	71.37	kJ/mol	Joback Method
log10ws	-7.59		Crippen Method
logp	5.848		Crippen Method
mcvol	247.340	ml/mol	McGowan Method
pc	1426.15	kPa	Joback Method
rinpol	1792.50		NIST Webbook
rinpol	1791.60		NIST Webbook
rinpol	1791.00		NIST Webbook
tb	794.10	K	Joback Method
tc	992.64	K	Joback Method
tf	489.48	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.30	J/mol×K	794.10	Joback Method
cpg	728.92	J/mol×K	827.19	Joback Method
cpg	741.61	J/mol×K	860.28	Joback Method
cpg	753.37	J/mol×K	893.37	Joback Method
cpg	764.23	J/mol×K	926.46	Joback Method
cpg	774.19	J/mol×K	959.55	Joback Method
cpg	783.27	J/mol×K	992.64	Joback Method

Sources

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=R433055&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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