3-Isopropylphenol, pentafluorobenzoyl ester

Inchi: InChI=1S/C16H11F5O2/c1-7(2)8-4-3-5-9(6-8)23-16(22)10-11(17)13(19)15(21)14(20)12(1
InchiKey: BOTYGERWLHEWNX-UHFFFAOYSA-N
Formula: C16H11F5O2
SMILES: CC(C)c1cccc(OC(=O)c2c(F)c(F)c(F)c(F)c2F)c1
Mol. weight [g/mol]: 330.25

Physical Properties

Property code	Value	Unit	Source
gf	-959.53	kJ/mol	Joback Method
hf	-1199.96	kJ/mol	Joback Method
hfus	37.61	kJ/mol	Joback Method
hvap	64.42	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	4.725		Crippen Method
mcvol	205.070	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
rinpol	1707.10		NIST Webbook
rinpol	1708.80		NIST Webbook
rinpol	1710.40		NIST Webbook
tb	720.92	K	Joback Method
tc	919.23	K	Joback Method
tf	458.15	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.85	J/mol×K	720.92	Joback Method
cpg	565.19	J/mol×K	753.97	Joback Method
cpg	576.75	J/mol×K	787.02	Joback Method
cpg	587.52	J/mol×K	820.08	Joback Method
cpg	597.52	J/mol×K	853.13	Joback Method
cpg	606.77	J/mol×K	886.18	Joback Method
cpg	615.26	J/mol×K	919.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R433184&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
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