

2-Isopropylphenol, pentafluorobenzoyl ester

Inchi:	InChI=1S/C16H11F5O2/c1-7(2)8-5-3-4-6-9(8)23-16(22)10-11(17)13(19)15(21)14(20)12(
InchiKey:	HFFGTHYNOHVNCV-UHFFFAOYSA-N
Formula:	C16H11F5O2
SMILES:	CC(C)c1ccccc1OC(=O)c1c(F)c(F)c(F)c(F)c1F
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	1648.00		NIST Webbook
rinpol	1651.20		NIST Webbook
rinpol	1649.30		NIST Webbook
rinpol	1648.00		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/molxK	720.92	Joback Method
cpg	565.19	J/molxK	753.97	Joback Method
cpg	576.75	J/molxK	787.02	Joback Method
cpg	587.52	J/molxK	820.08	Joback Method
cpg	597.52	J/molxK	853.13	Joback Method
cpg	606.77	J/molxK	886.18	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=R433080&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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