3-Methyl-4-isopropylphenol, pentafluorobenzoyl ester

Inchi: InChI=1S/C17H13F5O2/c1-7(2)10-5-4-9(6-8(10)3)24-17(23)11-12(18)14(20)16(22)15(21
InchiKey: HGXLRQZUZUHQJB-UHFFFAOYSA-N
Formula: C17H13F5O2
SMILES: Cc1cc(OC(=O)c2c(F)c(F)c(F)c(F)c2F)ccc1C(C)C
Mol. weight [g/mol]: 344.28

Physical Properties

Property code	Value	Unit	Source
gf	-960.74	kJ/mol	Joback Method
hf	-1232.07	kJ/mol	Joback Method
hfus	39.81	kJ/mol	Joback Method
hvap	67.30	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	5.033		Crippen Method
mcvol	219.160	ml/mol	McGowan Method
pc	1647.09	kPa	Joback Method
rinpol	1842.60		NIST Webbook
rinpol	1845.60		NIST Webbook
rinpol	1840.10		NIST Webbook
rinpol	1840.10		NIST Webbook
tb	748.78	K	Joback Method
tc	946.45	K	Joback Method
tf	481.94	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.92	J/mol×K	748.78	Joback Method
cpg	617.62	J/mol×K	781.73	Joback Method
cpg	629.50	J/mol×K	814.67	Joback Method
cpg	640.57	J/mol×K	847.62	Joback Method
cpg	650.84	J/mol×K	880.56	Joback Method
cpg	660.31	J/mol×K	913.51	Joback Method

cpg	669.00	J/mol×K	946.45	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=R433199&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