2-tert-Butyl-4-methylphenol, pentafluorobenzoyl ester

Inchi: InChI=1S/C18H15F5O2/c1-8-5-6-10(9(7-8)18(2,3)4)25-17(24)11-12(19)14(21)16(23)15(2

InchiKey: ZCRLHWKYPBPOAY-UHFFFAOYSA-N

Formula: C18H15F5O2

SMILES: Cc1ccc(OC(=O)c2c(F)c(F)c(F)c(F)c2F)c(C(C)(C)C)c1

Mol. weight [g/mol]: 358.30

Physical Properties

Property code	Value	Unit	Source
gf	-947.04	kJ/mol	Joback Method
hf	-1256.18	kJ/mol	Joback Method
hfus	38.51	kJ/mol	Joback Method
hvap	68.62	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	5.207		Crippen Method
mcvol	233.250	ml/mol	McGowan Method
pc	1539.08	kPa	Joback Method
rinpol	1812.40		NIST Webbook
rinpol	1809.50		NIST Webbook
rinpol	1806.60		NIST Webbook
tb	768.87	K	Joback Method
tc	970.14	K	Joback Method
tf	510.63	K	Joback Method
vc	0.930	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.79	J/mol×K	768.87	Joback Method
cpg	673.90	J/mol×K	802.42	Joback Method
cpg	686.12	J/mol×K	835.96	Joback Method
cpg	697.48	J/mol×K	869.51	Joback Method
cpg	708.00	J/mol×K	903.05	Joback Method
cpg	717.72	J/mol×K	936.60	Joback Method
cpg	726.65	J/mol×K	970.14	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R433124&Units=SI

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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