3-tert-Butylphenol, pentafluorobenzoyl ester

Inchi: InChI=1S/C17H13F5O2/c1-17(2,3)8-5-4-6-9(7-8)24-16(23)10-11(18)13(20)15(22)14(21)1
InchiKey: SKRLERIIIDOISA-UHFFFAOYSA-N
Formula: C17H13F5O2
SMILES: CC(C)(C)c1cccc(OC(=O)c2c(F)c(F)c(F)c(F)c2F)c1
Mol. weight [g/mol]: 344.28

Physical Properties

Property code	Value	Unit	Source
gf	-945.83	kJ/mol	Joback Method
hf	-1224.07	kJ/mol	Joback Method
hfus	36.31	kJ/mol	Joback Method
hvap	65.73	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	4.899		Crippen Method
mcvol	219.160	ml/mol	McGowan Method
pc	1682.41	kPa	Joback Method
rinpol	1759.40		NIST Webbook
rinpol	1761.10		NIST Webbook
rinpol	1763.00		NIST Webbook
rinpol	1759.40		NIST Webbook
tb	741.01	K	Joback Method
tc	942.96	K	Joback Method
tf	486.84	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	607.86	J/mol×K	741.01	Joback Method
cpg	620.68	J/mol×K	774.67	Joback Method
cpg	632.62	J/mol×K	808.33	Joback Method
cpg	643.72	J/mol×K	841.99	Joback Method
cpg	654.01	J/mol×K	875.65	Joback Method
cpg	663.51	J/mol×K	909.31	Joback Method

cpg	672.25	J/mol×K	942.96	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=R433228&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