4-sec-Butylphenol, pentafluorobenzoyl ester

Inchi: InChI=1S/C17H13F5O2/c1-3-8(2)9-4-6-10(7-5-9)24-17(23)11-12(18)14(20)16(22)15(21)1
InchiKey: HZOMKCOPLFCGAT-UHFFFAOYSA-N
Formula: C17H13F5O2
SMILES: CCC(C)c1ccc(OC(=O)c2c(F)c(F)c(F)c(F)c2F)cc1
Mol. weight [g/mol]: 344.28

Physical Properties

Property code	Value	Unit	Source
gf	-951.11	kJ/mol	Joback Method
hf	-1220.60	kJ/mol	Joback Method
hfus	40.20	kJ/mol	Joback Method
hvap	66.64	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	5.115		Crippen Method
mcvol	219.160	ml/mol	McGowan Method
pc	1667.33	kPa	Joback Method
rinpol	1830.50		NIST Webbook
rinpol	1823.60		NIST Webbook
rinpol	1823.60		NIST Webbook
rinpol	1826.70		NIST Webbook
tb	743.80	K	Joback Method
tc	940.66	K	Joback Method
tf	469.42	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.03	J/mol×K	743.80	Joback Method
cpg	618.82	J/mol×K	776.61	Joback Method
cpg	630.79	J/mol×K	809.42	Joback Method
cpg	641.93	J/mol×K	842.23	Joback Method
cpg	652.27	J/mol×K	875.04	Joback Method
cpg	661.82	J/mol×K	907.85	Joback Method

cpg	670.59	J/mol×K	940.66	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=R433337&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