4(1,1-Dimethylpentyl)phenol, pentafluorobenzoyl ester

Inchi: InChI=1S/C20H19F5O2/c1-4-5-10-20(2,3)11-6-8-12(9-7-11)27-19(26)13-14(21)16(23)18

InchiKey: CUYCNFQQLORCGW-UHFFFAOYSA-N

Formula: C20H19F5O2

SMILES: CCCCC(C)(C)c1ccc(OC(=O)c2c(F)c(F)c(F)c(F)c2F)cc1

Mol. weight [g/mol]: 386.36

Physical Properties

Property code	Value	Unit	Source
gf	-920.57	kJ/mol	Joback Method
hf	-1285.99	kJ/mol	Joback Method
hfus	44.08	kJ/mol	Joback Method
hvap	72.41	kJ/mol	Joback Method
log10ws	-7.79		Crippen Method
logp	6.069		Crippen Method
mcvol	261.430	ml/mol	McGowan Method
pc	1345.70	kPa	Joback Method
rinpol	2073.10		NIST Webbook
rinpol	2077.30		NIST Webbook
rinpol	2069.50		NIST Webbook
tb	809.65	K	Joback Method
tc	1008.82	K	Joback Method
tf	520.65	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	773.06	J/mol×K	809.65	Joback Method
cpg	786.92	J/mol×K	842.84	Joback Method
cpg	799.82	J/mol×K	876.04	Joback Method
cpg	811.81	J/mol×K	909.23	Joback Method
cpg	822.92	J/mol×K	942.43	Joback Method
cpg	833.18	J/mol×K	975.62	Joback Method
cpg	842.63	J/mol×K	1008.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R433288&Units=SI
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

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