4(1,2,2-Trimethylpropyl)phenol, pentafluorobenzoyl ester

Inchi: InChI=1S/C19H17F5O2/c1-9(19(2,3)4)10-5-7-11(8-6-10)26-18(25)12-13(20)15(22)17(24
InchiKey: RQUVJBSGNOEDPS-UHFFFAOYSA-N
Formula: C19H17F5O2
SMILES: CC(c1ccc(OC(=O)c2c(F)c(F)c(F)c(F)c2F)cc1)C(C)(C)C
Mol. weight [g/mol]: 372.33

Physical Properties

Property code	Value	Unit	Source
gf	-931.43	kJ/mol	Joback Method
hf	-1270.63	kJ/mol	Joback Method
hfus	37.96	kJ/mol	Joback Method
hvap	69.80	kJ/mol	Joback Method
log10ws	-7.42		Crippen Method
logp	5.751		Crippen Method
mcvol	247.340	ml/mol	McGowan Method
pc	1454.57	kPa	Joback Method
rinpol	2011.90		NIST Webbook
rinpol	2006.10		NIST Webbook
rinpol	2018.70		NIST Webbook
rinpol	2006.10		NIST Webbook
tb	786.33	K	Joback Method
tc	988.30	K	Joback Method
tf	494.38	K	Joback Method
vc	0.981	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.55	J/mol×K	786.33	Joback Method
cpg	731.26	J/mol×K	819.99	Joback Method
cpg	744.01	J/mol×K	853.65	Joback Method
cpg	755.83	J/mol×K	887.32	Joback Method
cpg	766.77	J/mol×K	920.98	Joback Method
cpg	776.85	J/mol×K	954.64	Joback Method

cpg	786.11	J/mol×K	988.30	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=R433317&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