4-n-Hexylphenol, pentafluorobenzoyl ester

Inchi: InChI=1S/C19H17F5O2/c1-2-3-4-5-6-11-7-9-12(10-8-11)26-19(25)13-14(20)16(22)18(24
InchiKey: KHSBSUDOQXFKNZ-UHFFFAOYSA-N
Formula: C19H17F5O2
SMILES: CCCCCCc1ccc(OC(=O)c2c(F)c(F)c(F)c(F)c2F)cc1
Mol. weight [g/mol]: 372.33

Physical Properties

Property code	Value	Unit	Source
gf	-931.83	kJ/mol	Joback Method
hf	-1256.60	kJ/mol	Joback Method
hfus	48.90	kJ/mol	Joback Method
hvap	71.48	kJ/mol	Joback Method
log10ws	-7.69		Crippen Method
logp	5.724		Crippen Method
mcvol	247.340	ml/mol	McGowan Method
pc	1425.07	kPa	Joback Method
rinpol	2082.40		NIST Webbook
rinpol	2075.20		NIST Webbook
rinpol	2078.60		NIST Webbook
rinpol	2075.20		NIST Webbook
tb	790.00	K	Joback Method
tc	983.50	K	Joback Method
tf	506.96	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.17	J/mol×K	790.00	Joback Method
cpg	728.58	J/mol×K	822.25	Joback Method
cpg	741.11	J/mol×K	854.50	Joback Method
cpg	752.78	J/mol×K	886.75	Joback Method
cpg	763.59	J/mol×K	919.00	Joback Method
cpg	773.58	J/mol×K	951.25	Joback Method

cpg	782.75	J/mol×K	983.50	Joback Method

Sources

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=R434474&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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