4-n-Pentylphenol, pentafluorobenzoyl ester

Inchi: InChI=1S/C18H15F5O2/c1-2-3-4-5-10-6-8-11(9-7-10)25-18(24)12-13(19)15(21)17(23)16
InchiKey: BIPGSYCSVJZLPI-UHFFFAOYSA-N
Formula: C18H15F5O2
SMILES: CCCCCc1ccc(OC(=O)c2c(F)c(F)c(F)c(F)c2F)cc1
Mol. weight [g/mol]: 358.30

Physical Properties

Property code	Value	Unit	Source
gf	-940.25	kJ/mol	Joback Method
hf	-1235.96	kJ/mol	Joback Method
hfus	46.31	kJ/mol	Joback Method
hvap	69.26	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	5.334		Crippen Method
mcvol	233.250	ml/mol	McGowan Method
pc	1534.26	kPa	Joback Method
rinpol	1973.00		NIST Webbook
rinpol	1979.70		NIST Webbook
rinpol	1976.30		NIST Webbook
rinpol	1973.00		NIST Webbook
tb	767.12	K	Joback Method
tc	960.70	K	Joback Method
tf	495.69	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.78	J/mol×K	767.12	Joback Method
cpg	672.81	J/mol×K	799.38	Joback Method
cpg	685.00	J/mol×K	831.65	Joback Method
cpg	696.37	J/mol×K	863.91	Joback Method
cpg	706.92	J/mol×K	896.17	Joback Method
cpg	716.68	J/mol×K	928.44	Joback Method

cpg	725.65	J/mol×K	960.70	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=R434503&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