4-n-Octylphenol, pentafluorobenzoyl ester

Inchi: InChI=1S/C21H21F5O2/c1-2-3-4-5-6-7-8-13-9-11-14(12-10-13)28-21(27)15-16(22)18(24
InchiKey: UHNTZIMKJXDBPJ-UHFFFAOYSA-N
Formula: C21H21F5O2
SMILES: CCCCCCCCc1ccc(OC(=O)c2c(F)c(F)c(F)c(F)c2F)cc1
Mol. weight [g/mol]: 400.38

Physical Properties

Property code	Value	Unit	Source
gf	-914.99	kJ/mol	Joback Method
hf	-1297.88	kJ/mol	Joback Method
hfus	54.08	kJ/mol	Joback Method
hvap	75.94	kJ/mol	Joback Method
log10ws	-8.53		Crippen Method
logp	6.504		Crippen Method
mcvol	275.520	ml/mol	McGowan Method
pc	1238.96	kPa	Joback Method
rinpol	2281.10		NIST Webbook
rinpol	2287.90		NIST Webbook
rinpol	2284.50		NIST Webbook
rinpol	2281.10		NIST Webbook
tb	835.76	K	Joback Method
tc	1031.00	K	Joback Method
tf	529.50	K	Joback Method
vc	1.109	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	828.81	J/mol×K	835.76	Joback Method
cpg	842.92	J/mol×K	868.30	Joback Method
cpg	856.06	J/mol×K	900.84	Joback Method
cpg	868.24	J/mol×K	933.38	Joback Method
cpg	879.50	J/mol×K	965.92	Joback Method
cpg	889.85	J/mol×K	998.46	Joback Method

cpg	899.31	J/mol×K	1031.00	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=R434494&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