4-n-Nonylphenol, pentafluorobenzoyl ester

Inchi: InChI=1S/C22H23F5O2/c1-2-3-4-5-6-7-8-9-14-10-12-15(13-11-14)29-22(28)16-17(23)19
InchiKey: JTXQZUCODJCZNY-UHFFFAOYSA-N
Formula: C22H23F5O2
SMILES: CCCCCCCCCc1ccc(OC(=O)c2c(F)c(F)c(F)c(F)c2F)cc1
Mol. weight [g/mol]: 414.41

Physical Properties

Property code	Value	Unit	Source
gf	-906.57	kJ/mol	Joback Method
hf	-1318.52	kJ/mol	Joback Method
hfus	56.67	kJ/mol	Joback Method
hvap	78.16	kJ/mol	Joback Method
log10ws	-8.95		Crippen Method
logp	6.894		Crippen Method
mcvol	289.610	ml/mol	McGowan Method
pc	1159.29	kPa	Joback Method
rinpol	2391.30		NIST Webbook
rinpol	2387.10		NIST Webbook
rinpol	2383.90		NIST Webbook
tb	858.64	K	Joback Method
tc	1055.82	K	Joback Method
tf	540.77	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.92	J/mol×K	858.64	Joback Method
cpg	901.36	J/mol×K	891.50	Joback Method
cpg	914.78	J/mol×K	924.37	Joback Method
cpg	927.20	J/mol×K	957.23	Joback Method
cpg	938.65	J/mol×K	990.10	Joback Method
cpg	949.14	J/mol×K	1022.96	Joback Method
cpg	958.71	J/mol×K	1055.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R434489&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