4-n-Heptylphenol, pentafluorobenzoyl ester

Inchi: InChI=1S/C20H19F5O2/c1-2-3-4-5-6-7-12-8-10-13(11-9-12)27-20(26)14-15(21)17(23)19
InchiKey: GPISQHZICIZRRM-UHFFFAOYSA-N
Formula: C20H19F5O2
SMILES: CCCCCCCc1ccc(OC(=O)c2c(F)c(F)c(F)c(F)c2F)cc1
Mol. weight [g/mol]: 386.36

Physical Properties

Property code	Value	Unit	Source
gf	-923.41	kJ/mol	Joback Method
hf	-1277.24	kJ/mol	Joback Method
hfus	51.49	kJ/mol	Joback Method
hvap	73.71	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	6.114		Crippen Method
mcvol	261.430	ml/mol	McGowan Method
pc	1327.14	kPa	Joback Method
rinpol	2185.20		NIST Webbook
rinpol	2181.80		NIST Webbook
rinpol	2178.40		NIST Webbook
rinpol	2178.40		NIST Webbook
tb	812.88	K	Joback Method
tc	1006.91	K	Joback Method
tf	518.23	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	771.54	J/mol×K	812.88	Joback Method
cpg	785.30	J/mol×K	845.22	Joback Method
cpg	798.15	J/mol×K	877.56	Joback Method
cpg	810.08	J/mol×K	909.90	Joback Method
cpg	821.13	J/mol×K	942.23	Joback Method
cpg	831.32	J/mol×K	974.57	Joback Method

cpg	840.65	J/mol×K	1006.91	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=R434469&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