3-n-Propylphenol, pentafluorobenzoyl ester

Inchi: InChI=1S/C16H11F5O2/c1-2-4-8-5-3-6-9(7-8)23-16(22)10-11(17)13(19)15(21)14(20)12(1
InchiKey: ZESUVBIIBZIUMO-UHFFFAOYSA-N
Formula: C16H11F5O2
SMILES: CCCc1cccc(OC(=O)c2c(F)c(F)c(F)c(F)c2F)c1
Mol. weight [g/mol]: 330.25

Physical Properties

Property code	Value	Unit	Source
gf	-957.09	kJ/mol	Joback Method
hf	-1194.68	kJ/mol	Joback Method
hfus	41.13	kJ/mol	Joback Method
hvap	64.81	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	4.554		Crippen Method
mcvol	205.070	ml/mol	McGowan Method
pc	1793.94	kPa	Joback Method
rinpol	1748.30		NIST Webbook
rinpol	1750.80		NIST Webbook
rinpol	1746.50		NIST Webbook
rinpol	1746.50		NIST Webbook
tb	721.36	K	Joback Method
tc	916.78	K	Joback Method
tf	473.15	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.28	J/mol×K	721.36	Joback Method
cpg	564.43	J/mol×K	753.93	Joback Method
cpg	575.82	J/mol×K	786.50	Joback Method
cpg	586.46	J/mol×K	819.07	Joback Method
cpg	596.36	J/mol×K	851.64	Joback Method
cpg	605.53	J/mol×K	884.21	Joback Method

cpg	613.98	J/mol×K	916.78	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=R433213&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