Pentafluorobenzoic acid, 2-propylphenyl ester

Other names: 2-n-Propylphenol, pentafluorobenzoyl ester
Inchi: InChI=1S/C16H11F5O2/c1-2-5-8-6-3-4-7-9(8)23-16(22)10-11(17)13(19)15(21)14(20)12(1
InchiKey: IEJFGMQLJBOJQU-UHFFFAOYSA-N
Formula: C16H11F5O2
SMILES: CCCc1ccccc1OC(=O)c1c(F)c(F)c(F)c(F)c1F
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	1688.00		NIST Webbook
rinpol	1685.90		NIST Webbook
rinpol	1707.00		NIST Webbook
rinpol	1690.70		NIST Webbook
rinpol	1707.00		NIST Webbook
rinpol	1685.90		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=U360627&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