2-Decenal, 4,5-epoxy, PFBO

Inchi: InChI=1S/C17H18F5NO2/c1-2-3-4-6-11-12(25-11)7-5-8-23-24-9-10-13(18)15(20)17(22)1
InchiKey: XWSHGXHSCROHSI-JNVYPNFTSA-N
Formula: C17H18F5NO2
SMILES: CCCCCC1OC1C=CC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 363.32

Physical Properties

Property code	Value	Unit	Source
hf	-1207.90	kJ/mol	Joback Method
hvap	64.73	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	4.788		Crippen Method
mcvol	237.740	ml/mol	McGowan Method
pc	1274.60	kPa	Joback Method
rinpol	2074.00		NIST Webbook
rinpol	2074.00		NIST Webbook
tb	768.57	K	Joback Method
tc	957.10	K	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=R398848&Units=SI

Legend

hf: Enthalpy of formation 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