(E,E)-2,4-Octadienal, PFBO # 2

Inchi: InChI=1S/C15H14F5NO/c1-2-3-4-5-6-7-8-21-22-9-10-11(16)13(18)15(20)14(19)12(10)17
InchiKey: BFLMIXVZQCNYHB-GQAZYRBESA-N
Formula: C15H14F5NO
SMILES: CCCC=CC=CC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 319.27

Physical Properties

Property code	Value	Unit	Source
hf	-969.86	kJ/mol	Joback Method
hvap	56.12	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	4.797		Crippen Method
mcvol	210.250	ml/mol	McGowan Method
pc	1429.38	kPa	Joback Method
rinpol	1797.00		NIST Webbook
tb	697.95	K	Joback Method
tc	883.43	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=R575694&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