(E)-2-Octenal, PFBO # 1

Inchi: InChI=1S/C15H16F5NO/c1-2-3-4-5-6-7-8-21-22-9-10-11(16)13(18)15(20)14(19)12(10)17
InchiKey: VUNPAXMYDAHBIY-PQEUULQISA-N
Formula: C15H16F5NO
SMILES: CCCCCC=CC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 321.29

Physical Properties

Property code	Value	Unit	Source
hf	-1087.08	kJ/mol	Joback Method
hvap	56.17	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	5.021		Crippen Method
mcvol	214.550	ml/mol	McGowan Method
pc	1374.80	kPa	Joback Method
rinpol	1711.00		NIST Webbook
rinpol	1723.00		NIST Webbook
rinpol	1711.00		NIST Webbook
ripol	2109.00		NIST Webbook
tb	693.79	K	Joback Method
tc	873.99	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R575525&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature