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

Inchi: InChI=1S/C14H12F5NO/c1-2-3-4-5-6-7-20-21-8-9-10(15)12(17)14(19)13(18)11(9)16/h3-
InchiKey: GAHPKCBQENDGSH-YDJHLNIVSA-N
Formula: C14H12F5NO
SMILES: CCC=CC=CC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 305.24

Physical Properties

Property code	Value	Unit	Source
hf	-949.22	kJ/mol	Joback Method
hvap	53.90	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	4.407		Crippen Method
mcvol	196.160	ml/mol	McGowan Method
pc	1539.08	kPa	Joback Method
rinpol	1694.00		NIST Webbook
ripol	2169.00		NIST Webbook
tb	675.07	K	Joback Method
tc	861.61	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=R575634&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature