(E)-2-Tridecenal, PFBO # 2

Inchi: InChI=1S/C20H26F5NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-26-27-14-15-16(21)18(23)20(25
InchiKey: PXSBSYDSKZOBAZ-JJWLEMJRSA-N
Formula: C20H26F5NO
SMILES: CCCCCCCCCCC=CC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 391.42

Physical Properties

Property code	Value	Unit	Source
hf	-1190.28	kJ/mol	Joback Method
hvap	67.30	kJ/mol	Joback Method
log10ws	-8.55		Crippen Method
logp	6.971		Crippen Method
mcvol	285.000	ml/mol	McGowan Method
pc	990.75	kPa	Joback Method
rinpol	2217.00		NIST Webbook
rinpol	2217.00		NIST Webbook
ripol	2612.00		NIST Webbook
ripol	2612.00		NIST Webbook
tb	808.19	K	Joback Method
tc	993.42	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R575570&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

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