(E)-2-Dodecenal, PFBO # 1

Inchi: InChI=1S/C19H24F5NO/c1-2-3-4-5-6-7-8-9-10-11-12-25-26-13-14-15(20)17(22)19(24)18
InchiKey: PFBICGCCBITBKY-CVWUSQQBSA-N
Formula: C19H24F5NO
SMILES: CCCCCCCCCC=CC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 377.39

Physical Properties

Property code	Value	Unit	Source
hf	-1169.64	kJ/mol	Joback Method
hvap	65.07	kJ/mol	Joback Method
log10ws	-8.13		Crippen Method
logp	6.581		Crippen Method
mcvol	270.910	ml/mol	McGowan Method
pc	1053.46	kPa	Joback Method
rinpol	2091.00		NIST Webbook
rinpol	2091.00		NIST Webbook
ripol	2501.00		NIST Webbook
ripol	2501.00		NIST Webbook
tb	785.31	K	Joback Method
tc	968.29	K	Joback Method

Sources

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=R575441&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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