Dodecanal, PFBO # 1

Inchi: InChI=1S/C19H26F5NO/c1-2-3-4-5-6-7-8-9-10-11-12-25-26-13-14-15(20)17(22)19(24)18
InchiKey: KVESFPFADCWDQR-UHFFFAOYSA-N
Formula: C19H26F5NO
SMILES: CCCCCCCCCCCC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 379.41

Physical Properties

Property code	Value	Unit	Source
hf	-1286.86	kJ/mol	Joback Method
hvap	65.11	kJ/mol	Joback Method
log10ws	-8.27		Crippen Method
logp	6.805		Crippen Method
mcvol	275.210	ml/mol	McGowan Method
pc	1018.78	kPa	Joback Method
rinpol	2040.00		NIST Webbook
rinpol	2040.00		NIST Webbook
ripol	2337.00		NIST Webbook
tb	781.15	K	Joback Method
tc	961.17	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R575387&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