2-Nonanone, PFBO # 2

Inchi: InChI=1S/C16H20F5NO/c1-3-4-5-6-7-8-10(2)22-23-9-11-12(17)14(19)16(21)15(20)13(11
InchiKey: NTPHAYZXDDTUAG-UHFFFAOYSA-N
Formula: C16H20F5NO
SMILES: CCCCCCCC(C)=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 337.33

Physical Properties

Property code	Value	Unit	Source
hf	-1234.73	kJ/mol	Joback Method
hvap	58.52	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	5.635		Crippen Method
mcvol	232.940	ml/mol	McGowan Method
pc	1239.83	kPa	Joback Method
rinpol	1683.00		NIST Webbook
rinpol	1683.00		NIST Webbook
ripol	1943.00		NIST Webbook
ripol	1943.00		NIST Webbook
tb	712.39	K	Joback Method
tc	889.65	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=R574804&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