2,3-Pentanedione, PFBO # 1

Inchi: InChI=1S/C19H12F10N2O2/c1-3-9(31-33-5-8-12(22)16(26)19(29)17(27)13(8)23)6(2)30-
InchiKey: QCZSYWXPYQVQDO-UHFFFAOYSA-N
Formula: C19H12F10N2O2
SMILES: CCC(=NOCc1c(F)c(F)c(F)c(F)c1F)C(C)=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 490.29

Physical Properties

Property code	Value	Unit	Source
hf	-2157.81	kJ/mol	Joback Method
hvap	72.50	kJ/mol	Joback Method
log10ws	-8.77		Crippen Method
logp	5.953		Crippen Method
mcvol	271.850	ml/mol	McGowan Method
pc	968.07	kPa	Joback Method
rinpol	1387.00		NIST Webbook
rinpol	1387.00		NIST Webbook
ripol	1812.00		NIST Webbook
ripol	1812.00		NIST Webbook
tb	927.94	K	Joback Method
tc	1136.13	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=R574606&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