n-Hexanal, O-[(pentafluorophenyl)methyl]oxime

Other names: Hexanal, PFBO, # 2
Inchi: InChI=1S/C13H14F5NO/c1-2-3-4-5-6-19-20-7-8-9(14)11(16)13(18)12(17)10(8)15/h6H,2-
InchiKey: GPAVMFOMYSGJDM-UHFFFAOYSA-N
Formula: C13H14F5NO
SMILES: CCCCCC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 295.25

Physical Properties

Property code	Value	Unit	Source
logp	4.465		Crippen Method
mcvol	190.670	ml/mol	McGowan Method
rinpol	1460.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1460.00		NIST Webbook
ripol	1765.00		NIST Webbook
ripol	1765.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U288098&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

ripol: Polar retention indices