2,4-Hexadienal oxime, O-[(pentafluorophenyl)methyl]-

Other names: (E,E)-2,4-Hexadienal, PFBO # 2
Inchi: InChI=1S/C13H10F5NO/c1-2-3-4-5-6-19-20-7-8-9(14)11(16)13(18)12(17)10(8)15/h2-6H,
InchiKey: LLOGYFAPZSCQBM-XKLQSORGSA-N
Formula: C13H10F5NO
SMILES: C/C=C/C=C/C=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 291.22

Physical Properties

Property code	Value	Unit	Source
logp	4.017		Crippen Method
mcvol	182.070	ml/mol	McGowan Method
rinpol	1599.00		NIST Webbook
ripol	2085.00		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=U288129&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