6-Methyl-5-hepten-2-one oxime, O-[(pentafluorophenyl)methyl]-

Other names: 6-Methyl-5-hepten-2-one, PFBO # 2
Inchi: InChI=1S/C15H16F5NO/c1-8(2)5-4-6-9(3)21-22-7-10-11(16)13(18)15(20)14(19)12(10)17
InchiKey: UNYXAVQWMIOYNJ-UHFFFAOYSA-N
Formula: C15H16F5NO
SMILES: CC(C)=CCCC(C)=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 321.29

Physical Properties

Property code	Value	Unit	Source
logp	5.021		Crippen Method
mcvol	214.550	ml/mol	McGowan Method
rinpol	1584.00		NIST Webbook
rinpol	1584.00		NIST Webbook
ripol	1883.00		NIST Webbook
ripol	1883.00		NIST Webbook

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U288124&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
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):

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

ripol: Polar retention indices