

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.cheméo.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

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