trans-2-Methyl-2-butenal oxime, O-[(pentafluorophenyl)methyl]-

Other names: (E)-2-Methyl-2-butenal, PFBO # 1
Inchi: InChI=1S/C12H10F5NO/c1-3-6(2)4-18-19-5-7-8(13)10(15)12(17)11(16)9(7)14/h3-4H,5H2
InchiKey: WEZKZVIRASBEJE-BDUDBEHWSA-N
Formula: C12H10F5NO
SMILES: C/C=C(\C)C=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 279.21

Physical Properties

Property code	Value	Unit	Source
logp	3.851		Crippen Method
mcvol	172.280	ml/mol	McGowan Method
rinpol	1493.00		NIST Webbook
rinpol	1493.00		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=U288144&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

Latest version available from: