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

Other names: Pentanal O-2,3,4,5,6-PFBHA-oxime
Pentanal, PFBO, # 2

Inchi: InChI=1S/C12H12F5NO/c1-2-3-4-5-18-19-6-7-8(13)10(15)12(17)11(16)9(7)14/h5H,2-4,6

InchiKey: CQVUQQBKUBLHIZ-UHFFFAOYSA-N

Formula: C12H12F5NO

SMILES: CCCCC=NOCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 281.22

Physical Properties

Property code	Value	Unit	Source
logp	4.075		Crippen Method
mcvol	176.580	ml/mol	McGowan Method
rinpol	1366.00		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1369.00		NIST Webbook
ripol	1675.00		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=C932710560&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