2-Furaldehyde O-pentafluorophenylmethyl-oxime

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

Inchi: InChI=1S/C12H6F5NO2/c13-8-7(9(14)11(16)12(17)10(8)15)5-20-18-4-6-2-1-3-19-6/h1-4

InchiKey: PLTMCEIKUMIAJJ-UHFFFAOYSA-N

Formula: C12H6F5NO2

SMILES: Fc1c(F)c(F)c(CON=Cc2ccco2)c(F)c1F

Mol. weight [g/mol]: 291.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.12		Crippen Method
logp	3.526		Crippen Method
mcvol	162.990	ml/mol	McGowan Method
rinpol	1510.00		NIST Webbook
rinpol	1510.00		NIST Webbook
ripol	2126.00		NIST Webbook
ripol	2126.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U372208&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

ripol: Polar retention indices