

# 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/ci9903071>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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

Latest version available from:

<https://www.cheméo.com/cid/121-726-1/2-Furaldehyde-O-pentafluorophenylmethyl-oxime.pdf>

Generated by Cheméo on 2024-04-30 15:01:04.726590376 +0000 UTC m=+16778513.647167688.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.