

Furfural, PFBO # 1

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	1491.00		NIST Webbook
rinpol	1491.00		NIST Webbook
ripol	2059.00		NIST Webbook
ripol	2059.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R575743&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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

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<https://www.chemeo.com/cid/125-018-3/Furfural-PFBO-1.pdf>

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