

# Isonicotinic acid, pentafluorobenzyl ester

**Inchi:** InChI=1S/C13H6F5NO2/c14-8-7(9(15)11(17)12(18)10(8)16)5-21-13(20)6-1-3-19-4-2-6/h  
**InchiKey:** ZUQWBMUCGXTFKU-UHFFFAOYSA-N  
**Formula:** C13H6F5NO2  
**SMILES:** O=C(OCc1c(F)c(F)c(F)c(F)c1F)c1ccncc1  
**Mol. weight [g/mol]:** 303.18

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.25		Crippen Method
logp	3.134		Crippen Method
mcvol	172.780	ml/mol	McGowan Method
rinpol	1690.00		NIST Webbook
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## Sources

**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=U376689&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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