

# Isonipecotic acid, N-pentafluorobenzoyl-, octyl ester

**Inchi:** InChI=1S/C21H26F5NO3/c1-2-3-4-5-6-7-12-30-21(29)13-8-10-27(11-9-13)20(28)14-15(2)  
**InchiKey:** FSNAQOUASCSMIP-UHFFFAOYSA-N  
**Formula:** C21H26F5NO3  
**SMILES:** CCCCCCOC(=O)C1CCN(C(=O)c2c(F)c(F)c(F)c(F)c2F)CC1  
**Mol. weight [g/mol]:** 435.43

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.81		Crippen Method
logp	5.138		Crippen Method
mcvol	299.970	ml/mol	McGowan Method
rinpol	2605.00		NIST Webbook
rinpol	2605.00		NIST Webbook

## 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=U361228&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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