

# Isonipecotic acid, N-(2,5-di(trifluoromethyl)benzoyl)-, octyl ester

**Inchi:** InChI=1S/C23H29F6NO3/c1-2-3-4-5-6-7-14-33-21(32)16-10-12-30(13-11-16)20(31)18-19  
**InchiKey:** MEUULPBSGZBDIH-UHFFFAOYSA-N  
**Formula:** C23H29F6NO3  
**SMILES:** CCCCCCOC(=O)C1CCN(C(=O)c2cc(C(F)(F)F)ccc2C(F)(F)F)CC1  
**Mol. weight [g/mol]:** 481.47

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.36		Crippen Method
logp	6.480		Crippen Method
mcvol	329.920	ml/mol	McGowan Method
rinpol	2570.00		NIST Webbook
rinpol	2570.00		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=U361208&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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