

# Isonipecotic acid, N-(3-bromobenzoyl)-, decyl ester

**Inchi:** InChI=1S/C23H34BrNO3/c1-2-3-4-5-6-7-8-9-17-28-23(27)19-13-15-25(16-14-19)22(26)2  
**InchiKey:** IMRRVRZISCFILF-UHFFFAOYSA-N  
**Formula:** C23H34BrNO3  
**SMILES:** CCCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(Br)c2)CC1  
**Mol. weight [g/mol]:** 452.43

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.15		Crippen Method
logp	5.985		Crippen Method
mcvol	336.800	ml/mol	McGowan Method
rinsol	3387.00		NIST Webbook
rinsol	3387.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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=U361518&Units=SI>

## Legend

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

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