

# Isonipecotic acid, n-butoxycarbonyl-, tetradecyl ester

**Inchi:** InChI=1S/C25H47NO4/c1-3-5-7-8-9-10-11-12-13-14-15-16-22-29-24(27)23-17-19-26(20-21)O  
**InchiKey:** VPRJXYABEPIRHL-UHFFFAOYSA-N  
**Formula:** C<sub>25</sub>H<sub>47</sub>NO<sub>4</sub>  
**SMILES:** CCCCCCCCCCCCCOC(=O)C1CCN(C(=O)OCCCC)CC1  
**Mol. weight [g/mol]:** 425.64

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.21		Crippen Method
logp	6.879		Crippen Method
mcvol	377.110	ml/mol	McGowan Method
rmpol	3281.00		NIST Webbook
rmpol	3281.00		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=U322058&Units=SI>

## Legend

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

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