

# Butoxyethyl nicotinate

**Other names:** nicoboxil  
**Inchi:** InChI=1S/C12H17NO3/c1-2-3-7-15-8-9-16-12(14)11-5-4-6-13-10-11/h4-6,10H,2-3,7-9H2  
**InchiKey:** IZJRISIINLJVBU-UHFFFAOYSA-N  
**Formula:** C12H17NO3  
**SMILES:** CCCCOCOC(=O)c1cccnc1  
**Mol. weight [g/mol]:** 223.27  
**CAS:** 13912-80-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.66		Crippen Method
logp	2.055		Crippen Method
mcvol	179.470	ml/mol	McGowan Method
rinpole	1640.00		NIST Webbook
rinpole	1640.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C13912806&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

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

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