

# p-Anisic acid, morpholide

**Inchi:** InChI=1S/C12H15NO3/c1-15-11-4-2-10(3-5-11)12(14)13-6-8-16-9-7-13/h2-5H,6-9H2,1H  
**InchiKey:** NQXDFSXYFLBDHX-UHFFFAOYSA-N  
**Formula:** C12H15NO3  
**SMILES:** COc1ccc(C(=O)N2CCOCC2)cc1  
**Mol. weight [g/mol]:** 221.25

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.55		Crippen Method
logp	1.168		Crippen Method
mcvol	168.610	ml/mol	McGowan Method
rinpol	1935.00		NIST Webbook
rinpol	1935.00		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=U307492&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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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