

o-Anisic acid, morpholide

Inchi: InChI=1S/C12H15NO3/c1-15-11-5-3-2-4-10(11)12(14)13-6-8-16-9-7-13/h2-5H,6-9H2,1H
InchiKey: ZCJLQRAZGYTKG-UHFFFAOYSA-N
Formula: C12H15NO3
SMILES: COc1ccccc1C(=O)N1CCOCC1
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
rinpola	1829.00		NIST Webbook
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Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U307055&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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