m-Anisic acid, morpholide

Inchi: InChI=1S/C12H15NO3/c1-15-11-4-2-3-10(9-11)12(14)13-5-7-16-8-6-13/h2-4,9H,5-8H2,1
InchiKey: RHNTVFHFVCLETB-UHFFFAOYSA-N
Formula: C12H15NO3
SMILES: COc1cccc(C(=O)N2CCOCC2)c1
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	1897.00		NIST Webbook
rinpol	1897.00		NIST Webbook

Sources

Crippen Method: 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=U306965&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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