

Isonicotinamide, N-(2,5-dimethoxyphenyl)-

Inchi: InChI=1S/C14H14N2O3/c1-18-11-3-4-13(19-2)12(9-11)16-14(17)10-5-7-15-8-6-10/h3-9H
InchiKey: FVROKLSMNJEOPA-UHFFFAOYSA-N
Formula: C14H14N2O3
SMILES: COc1ccc(OC)c(NC(=O)c2ccncc2)c1
Mol. weight [g/mol]: 258.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.45		Crippen Method
logp	2.351		Crippen Method
mcvol	193.870	ml/mol	McGowan Method
rinpol	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U307416&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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