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

Inchi:	InChI=1S/C14H14N2O3/c1-18-11-5-6-13(19-2)12(8-11)16-14(17)10-4-3-7-15-9-10/h3-9H
InchiKey:	JTFFVIBKHIYKCR-UHFFFAOYSA-N
Formula:	C14H14N2O3
SMILES:	COc1ccc(OC)c(NC(=O)c2cccnc2)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	2334.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308109&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	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
rinpol:	Non-polar retention indices

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