

Isonicotinamide, N-(4-methoxyphenyl)-

Inchi: InChI=1S/C13H12N2O2/c1-17-12-4-2-11(3-5-12)15-13(16)10-6-8-14-9-7-10/h2-9H,1H3,
InchiKey: LVERVLNIJMUPKJ-UHFFFAOYSA-N
Formula: C13H12N2O2
SMILES: COc1ccc(NC(=O)c2ccncc2)cc1
Mol. weight [g/mol]: 228.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.33		Crippen Method
logp	2.342		Crippen Method
mcvol	173.910	ml/mol	McGowan Method
rinpola	2217.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U307414&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
rinpola: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/25-793-4/Isonicotinamide-N-4-methoxyphenyl.pdf>

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