Nicotinamide, N-(4-methoxyphenyl)-

Inchi: InChI=1S/C13H12N2O2/c1-17-12-6-4-11(5-7-12)15-13(16)10-3-2-8-14-9-10/h2-9H,1H3,(
InchiKey: BIIGKWRZEOUZSI-UHFFFAOYSA-N
Formula: C13H12N2O2
SMILES: COc1ccc(NC(=O)c2cccnc2)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
rinpol	2250.00		NIST Webbook
rinpol	2250.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U308107&Units=SI

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.