2-Furancarboxamide, N-(4-methoxyphenyl)-

Inchi: InChI=1S/C12H11NO3/c1-15-10-6-4-9(5-7-10)13-12(14)11-3-2-8-16-11/h2-8H,1H3,(H,13
InchiKey: BAPQOHAPCRWHRC-UHFFFAOYSA-N
Formula: C12H11NO3
SMILES: COc1ccc(NC(=O)c2ccco2)cc1
Mol. weight [g/mol]: 217.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.30		Crippen Method
logp	2.540		Crippen Method
mcvol	160.010	ml/mol	McGowan Method
rinpol	1982.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307038&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