

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
rinsol	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/ci990307I
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
rinsol:	Non-polar retention indices

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<https://www.chemeo.com/cid/45-939-0/2-Furancarboxamide-N-4-methoxyphenyl.pdf>

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