2-Furoic acid, 4-methoxyphenyl ester

Inchi: InChI=1S/C12H10O4/c1-14-9-4-6-10(7-5-9)16-12(13)11-3-2-8-15-11/h2-8H,1H3
InchiKey: PUIKCDWMCVPTGK-UHFFFAOYSA-N
Formula: C12H10O4
SMILES: COc1ccc(OC(=O)c2ccco2)cc1
Mol. weight [g/mol]: 218.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.41		Crippen Method
logp	2.507		Crippen Method
mcvol	155.900	ml/mol	McGowan Method
rinpol	1759.00		NIST Webbook

Sources

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=U307995&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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