2-Furoic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C13H12O3/c1-9-6-10(2)8-11(7-9)16-13(14)12-4-3-5-15-12/h3-8H,1-2H3
InchiKey: OVMWSUWVYAXNGM-UHFFFAOYSA-N
Formula: C13H12O3
SMILES: Cc1cc(C)cc(OC(=O)c2ccco2)c1
Mol. weight [g/mol]: 216.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.24		Crippen Method
logp	3.116		Crippen Method
mcvol	164.120	ml/mol	McGowan Method
rinpol	1706.00		NIST Webbook
rinpol	1706.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307994&Units=SI
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

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.