2-Furoic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C12H7NO3/c13-8-9-3-5-10(6-4-9)16-12(14)11-2-1-7-15-11/h1-7H
InchiKey: YYLGZLHCYFGOTM-UHFFFAOYSA-N
Formula: C12H7NO3
SMILES: N#Cc1ccc(OC(=O)c2ccco2)cc1
Mol. weight [g/mol]: 213.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.64		Crippen Method
logp	2.370		Crippen Method
mcvol	151.410	ml/mol	McGowan Method
rinpol	1792.00		NIST Webbook
rinpol	1792.00		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=U307996&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.