2-Furoic acid, 2-naphthyl ester

Inchi: InChI=1S/C15H10O3/c16-15(14-6-3-9-17-14)18-13-8-7-11-4-1-2-5-12(11)10-13/h1-10H
InchiKey: DDSZKPNUXDONMN-UHFFFAOYSA-N
Formula: C15H10O3
SMILES: O=C(Oc1ccc2ccccc2c1)c1ccco1
Mol. weight [g/mol]: 238.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.10		Crippen Method
logp	3.652		Crippen Method
mcvol	172.840	ml/mol	McGowan Method
rinpol	2087.00		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=U307999&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