

2-Furoic acid, undec-2-enyl ester

Inchi: InChI=1S/C16H24O3/c1-2-3-4-5-6-7-8-9-10-13-19-16(17)15-12-11-14-18-15/h9-12,14H,2
InchiKey: XAVQJBRHRAITNF-MDZDMXLPSA-N
Formula: C16H24O3
SMILES: CCCCCCCC=CCOC(=O)c1ccc1
Mol. weight [g/mol]: 264.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.49		Crippen Method
logp	4.743		Crippen Method
mcvol	225.850	ml/mol	McGowan Method
rinpol	1938.00		NIST Webbook
rinpol	1938.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U299240&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

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