2-Furoic acid, oct-3-en-2-yl ester

Inchi: InChI=1S/C13H18O3/c1-3-4-5-6-8-11(2)16-13(14)12-9-7-10-15-12/h6-11H,3-5H2,1-2H3/
InchiKey: NDCBQSHNDZHGPS-SOFGYWHQSA-N
Formula: C13H18O3
SMILES: CCCCC=CC(C)OC(=O)c1ccco1
Mol. weight [g/mol]: 222.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.34		Crippen Method
logp	3.571		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
rinpol	1539.00		NIST Webbook
rinpol	1539.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299236&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.