

2-Furoic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C18H26O3/c1-2-3-4-5-6-7-8-9-10-11-12-15-21-18(19)17-14-13-16-20-17/h13-14
InchiKey: XSTWMTSBFZQZRB-UHFFFAOYSA-N
Formula: C18H26O3
SMILES: CCCCCCCCCC#CCOC(=O)c1ccc1
Mol. weight [g/mol]: 290.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.27		Crippen Method
logp	4.971		Crippen Method
mcvol	249.730	ml/mol	McGowan Method
rinpol	2156.00		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=U299241&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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<https://www.chemeo.com/cid/41-940-2/2-Furoic-acid-tridec-2-ynyl-ester.pdf>

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