2-Furoic acid, 8-chlorooctyl ester

Inchi: InChI=1S/C13H19ClO3/c14-9-5-3-1-2-4-6-10-17-13(15)12-8-7-11-16-12/h7-8,11H,1-6,9-1
InchiKey: GRSYGFYMCIAFNY-UHFFFAOYSA-N
Formula: C13H19ClO3
SMILES: O=C(OCCCCCCCCCCl)c1ccco1
Mol. weight [g/mol]: 258.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.53		Crippen Method
logp	4.016		Crippen Method
mcvol	200.120	ml/mol	McGowan Method
rinpol	2004.00		NIST Webbook
rinpol	2004.00		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=U355174&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.