Methyl 8-(2-furyl)octanoate

Other names: Octanoic acid, 8-(2-furyl), methyl ester
Inchi: InChI=1S/C13H20O3/c1-15-13(14)10-6-4-2-3-5-8-12-9-7-11-16-12/h7,9,11H,2-6,8,10H2,
InchiKey: BEDHFJANVUDDFI-UHFFFAOYSA-N
Formula: C13H20O3
SMILES: COC(=O)CCCCCCCc1ccco1
Mol. weight [g/mol]: 224.30
CAS: 38199-50-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.80		Crippen Method
logp	3.336		Crippen Method
mcvol	187.880	ml/mol	McGowan Method
rinpol	1629.00		NIST Webbook
rinpol	1624.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1624.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1629.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C38199507&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices