Methyl 7-(2-furoyl)heptanoate

Other names: Octanoic acid, 8-oxo-8-(2-furyl), ethyl ester
Inchi: InChI=1S/C13H18O4/c1-16-13(15)9-5-3-2-4-7-11(14)12-8-6-10-17-12/h6,8,10H,2-5,7,9H
InchiKey: YEJWQYJOGFNXRR-UHFFFAOYSA-N
Formula: C13H18O4
SMILES: COC(=O)CCCCCCC(=O)c1ccco1
Mol. weight [g/mol]: 238.28
CAS: 38199-47-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.66		Crippen Method
logp	2.976		Crippen Method
mcvol	189.450	ml/mol	McGowan Method
rinpol	1920.00		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=C38199472&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

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