Furan, 2-decanoyl

Inchi: InChI=1S/C14H22O2/c1-2-3-4-5-6-7-8-10-13(15)14-11-9-12-16-14/h9,11-12H,2-8,10H2,1
InchiKey: RPZFIMHVHRPTRD-UHFFFAOYSA-N
Formula: C14H22O2
SMILES: CCCCCCCCCC(=O)c1ccco1
Mol. weight [g/mol]: 222.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.21		Crippen Method
logp	4.603		Crippen Method
mcvol	196.100	ml/mol	McGowan Method
rinpol	1689.00		NIST Webbook
rinpol	1689.00		NIST Webbook
ripol	2264.00		NIST Webbook
ripol	2264.00		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=R409864&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
ripol: Polar retention indices

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