

Furan, 2-nonanoyl

Inchi: InChI=1S/C13H20O2/c1-2-3-4-5-6-7-9-12(14)13-10-8-11-15-13/h8,10-11H,2-7,9H2,1H3
InchiKey: IVMLTMNCNAILQF-UHFFFAOYSA-N
Formula: C13H20O2
SMILES: CCCCCCCCC(=O)c1ccco1
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.80		Crippen Method
logp	4.213		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
rinpol	1588.00		NIST Webbook
rinpol	1588.00		NIST Webbook
ripol	2163.00		NIST Webbook
ripol	2163.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R409879&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
ripol: Polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/90-763-5/Furan-2-nonanoyl.pdf>

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