

# Furfuryl hexanoate

<b>Other names:</b>	Furfuryl n-hexanoate Hexanoic acid, 2-furanylmethyl ester furan-2-ylmethyl hexanoate
<b>Inchi:</b>	InChI=1S/C11H16O3/c1-2-3-4-7-11(12)14-9-10-6-5-8-13-10/h5-6,8H,2-4,7,9H2,1H3
<b>InchiKey:</b>	IBIDUABZZSJJNF-UHFFFAOYSA-N
<b>Formula:</b>	C11H16O3
<b>SMILES:</b>	CCCCC(=O)OCc1ccco1
<b>Mol. weight [g/mol]:</b>	196.24
<b>CAS:</b>	39252-02-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.46		Crippen Method
logp	2.903		Crippen Method
mcvol	159.700	ml/mol	McGowan Method
ripol	1368.00		NIST Webbook
ripol	1368.00		NIST Webbook
ripol	1368.00		NIST Webbook
ripol	1343.00		NIST Webbook
ripol	1857.00		NIST Webbook
ripol	1850.00		NIST Webbook

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C39252023&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C39252023&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices

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