

# 2-Furancarboxylic acid, 3-methylbutyl ester

<b>Other names:</b>	iso-Amyl 2-furoate Isoamyl furoate 2-Furoic acid, 3-methylbutyl ester 3-methylbutyl 2-furoate
<b>Inchi:</b>	InChI=1S/C10H14O3/c1-8(2)5-7-13-10(11)9-4-3-6-12-9/h3-4,6,8H,5,7H2,1-2H3
<b>InchiKey:</b>	FPBZWZKAUPNMMV-UHFFFAOYSA-N
<b>Formula:</b>	C10H14O3
<b>SMILES:</b>	CC(C)CCOC(=O)c1ccco1
<b>Mol. weight [g/mol]:</b>	182.22
<b>CAS:</b>	615-12-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.88		Crippen Method
logp	2.482		Crippen Method
mcvol	145.610	ml/mol	McGowan Method
rinpol	1318.00		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1287.00		NIST Webbook
ripol	1840.00		NIST Webbook
ripol	1840.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C615123&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C615123&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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