

# 2-Furanpropanoic acid, 3-methylbutyl ester

<b>Other names:</b>	iso-Amyl furylpropionate 3-methylbutyl furan-2-propionate
<b>Inchi:</b>	InChI=1S/C12H18O3/c1-10(2)7-9-15-12(13)6-5-11-4-3-8-14-11/h3-4,8,10H,5-7,9H2,1-2H
<b>InchiKey:</b>	ZVMWAVZRUZDYMV-UHFFFAOYSA-N
<b>Formula:</b>	C12H18O3
<b>SMILES:</b>	CC(C)CCOC(=O)CCc1ccco1
<b>Mol. weight [g/mol]:</b>	210.27
<b>CAS:</b>	7779-67-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.14		Crippen Method
logp	2.801		Crippen Method
mcvol	173.790	ml/mol	McGowan Method
rinpol	1415.00		NIST Webbook
ripol	1894.00		NIST Webbook
ripol	1894.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C7779671&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7779671&amp;Units=SI</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

**ripol:**

Polar retention indices

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