

Butanoic acid, 3-methyl-, 2-furanylmethyl ester

Other names:	Furfuryl 3-methylbutanoate Furfuryl isovalerate
Inchi:	InChI=1S/C10H14O3/c1-8(2)6-10(11)13-7-9-4-3-5-12-9/h3-5,8H,6-7H2,1-2H3
InchiKey:	FKGUIBCHHSHJNQ-UHFFFAOYSA-N
Formula:	C10H14O3
SMILES:	CC(C)CC(=O)OCc1cccO1
Mol. weight [g/mol]:	182.22
CAS:	13678-60-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.80		Crippen Method
logp	2.369		Crippen Method
mcvol	145.610	ml/mol	McGowan Method
rinpol	1223.70		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1222.00		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=C13678609&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

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