

Butanoic acid, 2-furanylmethyl ester

Other names:	Butyric acid, furfuryl ester Furfuryl butyrate Furfuryl n-butyrate 2-Furfuryl butyrate 2-Furfuryl n-butyrate Furfuryl butanoate
Inchi:	InChI=1S/C9H12O3/c1-2-4-9(10)12-7-8-5-3-6-11-8/h3,5-6H,2,4,7H2,1H3
InchiKey:	IXISGRHWGVGCAK-UHFFFAOYSA-N
Formula:	C9H12O3
SMILES:	CCCC(=O)OCc1ccco1
Mol. weight [g/mol]:	168.19
CAS:	623-21-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.62		Crippen Method
logp	2.123		Crippen Method
mcvol	131.520	ml/mol	McGowan Method
rinpol	1171.00		NIST Webbook
rinpol	1148.00		NIST Webbook
ripol	1649.00		NIST Webbook
ripol	1649.00		NIST Webbook
ripol	1655.00		NIST Webbook
ripol	1665.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C623212&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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