

Butyl 3-furylpropanoate

Inchi:	InChI=1S/C11H16O3/c1-2-3-7-14-11(12)5-4-10-6-8-13-9-10/h6,8-9H,2-5,7H2,1H3
InchiKey:	GKBPVNJYWGTECJ-UHFFFAOYSA-N
Formula:	C11H16O3
SMILES:	CCCCOC(=O)CCc1ccoc1
Mol. weight [g/mol]:	196.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.96		Crippen Method
logp	2.555		Crippen Method
mcvol	159.700	ml/mol	McGowan Method
rinpol	1354.00		NIST Webbook
rinpol	1354.00		NIST Webbook
ripol	1728.00		NIST Webbook
ripol	1728.00		NIST Webbook

Sources

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=R508000&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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