

Sarcosine, N-(2-furoyl)-, isobutyl ester

Inchi:	InChI=1S/C12H17NO4/c1-9(2)8-17-11(14)7-13(3)12(15)10-5-4-6-16-10/h4-6,9H,7-8H2,1
InchiKey:	OMDXFERPDICUIV-UHFFFAOYSA-N
Formula:	C12H17NO4
SMILES:	CC(C)COC(=O)CN(C)C(=O)c1ccco1
Mol. weight [g/mol]:	239.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.06		Crippen Method
logp	1.551		Crippen Method
mcvol	185.340	ml/mol	McGowan Method
rinpol	1780.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321433&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

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<https://www.chemeo.com/cid/44-074-1/Sarcosine-N-2-furoyl-isobutyl-ester.pdf>

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