

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

Inchi:	InChI=1S/C10H13NO4/c1-3-14-9(12)7-11(2)10(13)8-5-4-6-15-8/h4-6H,3,7H2,1-2H3
InchiKey:	OJVYTBUDKHOIEP-UHFFFAOYSA-N
Formula:	C10H13NO4
SMILES:	CCOC(=O)CN(C)C(=O)c1ccco1
Mol. weight [g/mol]:	211.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.47		Crippen Method
logp	0.915		Crippen Method
mcvol	157.160	ml/mol	McGowan Method
rinpol	1637.00		NIST Webbook
rinpol	1637.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U321431&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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<https://www.cheméo.com/cid/19-884-0/Sarcosine-N-2-furoyl-ethyl-ester.pdf>

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