

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

Inchi:	InChI=1S/C19H31NO4/c1-3-4-5-6-7-8-9-10-11-14-24-18(21)16-20(2)19(22)17-13-12-15-
InchiKey:	DFMQEDVFAQDMCO-UHFFFAOYSA-N
Formula:	C19H31NO4
SMILES:	CCCCCCCCCOC(=O)CN(C)C(=O)c1ccco1
Mol. weight [g/mol]:	337.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.23		Crippen Method
logp	4.426		Crippen Method
mcvol	283.970	ml/mol	McGowan Method
rinpol	2539.00		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=U321441&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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