

Furan-2-carboxamide, N-butyl-N-nonyl-

Inchi:	InChI=1S/C18H31NO2/c1-3-5-7-8-9-10-11-15-19(14-6-4-2)18(20)17-13-12-16-21-17/h12
InchiKey:	KWZIIYIXTLIKANN-UHFFFAOYSA-N
Formula:	C18H31NO2
SMILES:	CCCCCCCCCN(CCCC)C(=O)c1ccco1
Mol. weight [g/mol]:	293.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.95		Crippen Method
logp	5.272		Crippen Method
mcvol	262.440	ml/mol	McGowan Method
rinpol	2837.00		NIST Webbook
rinpol	2837.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415649&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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