

Furan-2-carboxamide, N-butyl-N-ethyl-

Inchi:	InChI=1S/C11H17NO2/c1-3-5-8-12(4-2)11(13)10-7-6-9-14-10/h6-7,9H,3-5,8H2,1-2H3
InchiKey:	MEHIAHYVJLGEHZ-UHFFFAOYSA-N
Formula:	C11H17NO2
SMILES:	CCCCN(CC)C(=O)c1ccco1
Mol. weight [g/mol]:	195.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.02		Crippen Method
logp	2.542		Crippen Method
mcvol	163.810	ml/mol	McGowan Method
rinpol	1749.00		NIST Webbook
rinpol	1749.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415640&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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