

Furan-2-carboxamide, N-butyl-N-2-ethylhexyl-

Inchi:	InChI=1S/C17H29NO2/c1-4-7-10-15(6-3)14-18(12-8-5-2)17(19)16-11-9-13-20-16/h9,11,1
InchiKey:	VYZPOJGFFKKALD-UHFFFAOYSA-N
Formula:	C17H29NO2
SMILES:	CCCCC(CC)CN(CCCC)C(=O)c1ccco1
Mol. weight [g/mol]:	279.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.29		Crippen Method
logp	4.738		Crippen Method
mcvol	248.350	ml/mol	McGowan Method
rinpol	2357.00		NIST Webbook
rinpol	2357.00		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=U415646&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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