Isonicotinamide, N,N-dibutyl-

Inchi: InChI=1S/C14H22N2O/c1-3-5-11-16(12-6-4-2)14(17)13-7-9-15-10-8-13/h7-10H,3-6,11-1
InchiKey: WTHCSKNSBMUVJX-UHFFFAOYSA-N
Formula: C14H22N2O
SMILES: CCCCN(CCCC)C(=O)c1ccncc1
Mol. weight [g/mol]: 234.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.89		Crippen Method
logp	3.124		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
rinpol	1808.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U308640&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