

Furan-2-carboxamide, N-butyl-N-dodecyl-

Inchi: InChI=1S/C21H37NO2/c1-3-5-7-8-9-10-11-12-13-14-18-22(17-6-4-2)21(23)20-16-15-19-7
InchiKey: PMVAXGSLGOTNPH-UHFFFAOYSA-N
Formula: C₂₁H₃₇NO₂
SMILES: CCCCCCCCCCCN(CCCC)C(=O)c1ccco1
Mol. weight [g/mol]: 335.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.21		Crippen Method
logp	6.443		Crippen Method
mcvol	304.710	ml/mol	McGowan Method
rinpol	3241.00		NIST Webbook
rinpol	3241.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U415652&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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