

Furan-2-carboxamide, N-butyl-N-3-methylbutyl-

Inchi: InChI=1S/C14H23NO2/c1-4-5-9-15(10-8-12(2)3)14(16)13-7-6-11-17-13/h6-7,11-12H,4-5
InchiKey: YJUOKZQHYHLHDV-UHFFFAOYSA-N
Formula: C14H23NO2
SMILES: CCCCNC(CCC(C)C)C(=O)c1ccco1
Mol. weight [g/mol]: 237.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.04		Crippen Method
logp	3.568		Crippen Method
mcvol	206.080	ml/mol	McGowan Method
rinpol	2177.00		NIST Webbook
rinpol	2177.00		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=U415644&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/117-597-0/Furan-2-carboxamide-N-butyl-N-3-methylbutyl.pdf>

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