2-Furancarboxamide, N-(3-methylbutyl)-

Inchi:	InChI=1S/C10H15NO2/c1-8(2)5-6-11-10(12)9-4-3-7-13-9/h3-4,7-8H,5-6H2,1-2H3,(H,11,1
InchiKey:	SXMDNBVBCUXKHP-UHFFFAOYSA-N
Formula:	C10H15NO2
SMILES:	CC(C)CCNC(=O)c1ccco1
Mol. weight [g/mol]:	181.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.98		Crippen Method
logp	2.055		Crippen Method
mcvol	149.720	ml/mol	McGowan Method
rinpol	1526.00		NIST Webbook
rinpol	1526.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407242&Units=SI
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

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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