

Isonipecotic acid, N-(4-methylbenzoyl)-, butyl ester

Inchi:	InChI=1S/C18H25NO3/c1-3-4-13-22-18(21)16-9-11-19(12-10-16)17(20)15-7-5-14(2)6-8-
InchiKey:	BUCAXIHWQXYNQU-UHFFFAOYSA-N
Formula:	C18H25NO3
SMILES:	CCCCOC(=O)C1CCN(C(=O)c2ccc(C)cc2)CC1
Mol. weight [g/mol]:	303.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.96		Crippen Method
logp	3.191		Crippen Method
mcvol	248.850	ml/mol	McGowan Method
rinpol	2578.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U361115&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

Latest version available from:

<https://www.cheméo.com/cid/14-026-7/Isonipecotic-acid-N-4-methylbenzoyl-butyl-ester.pdf>

Generated by Cheméo on 2024-04-28 07:39:19.183328587 +0000 UTC m=+16579208.103905900.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.