

Isonipecotic acid, N-(3-methoxybenzoyl)-, butyl ester

Inchi: InChI=1S/C18H25NO4/c1-3-4-12-23-18(21)14-8-10-19(11-9-14)17(20)15-6-5-7-16(13-15)
InchiKey: UTALXVBGHLMXKG-UHFFFAOYSA-N
Formula: C18H25NO4
SMILES: CCCOC(=O)C1CCN(C(=O)c2cccc(OC)c2)CC1
Mol. weight [g/mol]: 319.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.60		Crippen Method
logp	2.891		Crippen Method
mcvol	254.720	ml/mol	McGowan Method
rinpole	2691.00		NIST Webbook
rinpole	2691.00		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=U361175&Units=SI>

Legend

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

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