

Isonipecotic acid, N-(4-nitrobenzoyl)-, isobutyl ester

Inchi:	InChI=1S/C17H22N2O5/c1-12(2)11-24-17(21)14-7-9-18(10-8-14)16(20)13-3-5-15(6-4-13)
InchiKey:	FSQCMADAPFRNKO-UHFFFAOYSA-N
Formula:	C17H22N2O5
SMILES:	CC(C)COC(=O)C1CCN(C(=O)c2ccc([N+](=O)[O-])cc2)CC1
Mol. weight [g/mol]:	334.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.89		Crippen Method
logp	2.646		Crippen Method
mcvol	252.180	ml/mol	McGowan Method
rmpol	2862.00		NIST Webbook
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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=U361042&Units=SI

Legend

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

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