

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

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

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.13		Crippen Method
logp	2.790		Crippen Method
mcvol	252.180	ml/mol	McGowan Method
rinpole	2918.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361043&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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