

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

Inchi:	InChI=1S/C18H24N2O5/c1-2-3-4-13-25-18(22)15-9-11-19(12-10-15)17(21)14-5-7-16(8-6
InchiKey:	ZKBANJRFEMMCAB-UHFFFAOYSA-N
Formula:	C18H24N2O5
SMILES:	CCCCCOC(=O)C1CCN(C(=O)c2ccc([N+](=O)[O-])cc2)CC1
Mol. weight [g/mol]:	348.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.55		Crippen Method
logp	3.180		Crippen Method
mcvol	266.270	ml/mol	McGowan Method
rinpola	3035.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.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=U361044&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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