

# Isonipecotic acid, N-(4-nitrobenzoyl)-, heptyl ester

Inchi:	InChI=1S/C20H28N2O5/c1-2-3-4-5-6-15-27-20(24)17-11-13-21(14-12-17)19(23)16-7-9-1
InchiKey:	JFILZDGJWQTVJE-UHFFFAOYSA-N
Formula:	C20H28N2O5
SMILES:	CCCCCCCOC(=O)C1CCN(C(=O)c2ccc([N+](=O)[O-])cc2)CC1
Mol. weight [g/mol]:	376.45

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.39		Crippen Method
logp	3.961		Crippen Method
mcvol	294.450	ml/mol	McGowan Method
rinpol	3251.00		NIST Webbook

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U361047&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361047&amp;Units=SI</a>

## Legend

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

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