

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

Inchi:	InChI=1S/C19H26N2O5/c1-14(2)4-3-13-26-19(23)16-9-11-20(12-10-16)18(22)15-5-7-17
InchiKey:	VQXTTXGLQONOPV-UHFFFAOYSA-N
Formula:	C19H26N2O5
SMILES:	CC(C)CCCOC(=O)C1CCN(C(=O)c2ccc([N+](=O)[O-])cc2)CC1
Mol. weight [g/mol]:	362.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.73		Crippen Method
logp	3.426		Crippen Method
mcvol	280.360	ml/mol	McGowan Method
rinpola	3103.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361045&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
mcvola:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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