

Isonipectic acid, N-(4-nitrobenzoyl)-, octyl ester

Inchi:	InChI=1S/C21H30N2O5/c1-2-3-4-5-6-7-16-28-21(25)18-12-14-22(15-13-18)20(24)17-8-1
InchiKey:	HGWBEPOMMROTNU-UHFFFAOYSA-N
Formula:	C21H30N2O5
SMILES:	CCCCCCCCOC(=O)C1CCN(C(=O)c2ccc([N+](=O)[O-])cc2)CC1
Mol. weight [g/mol]:	390.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.80		Crippen Method
logp	4.351		Crippen Method
mcvol	308.540	ml/mol	McGowan Method
rinsol	3353.00		NIST Webbook
rinsol	3353.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361048&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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