

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

Inchi:	InChI=1S/C15H18N2O5/c1-2-22-15(19)12-7-9-16(10-8-12)14(18)11-3-5-13(6-4-11)17(20)
InchiKey:	SFUOAIRNUIFKPE-UHFFFAOYSA-N
Formula:	C15H18N2O5
SMILES:	CCOC(=O)C1CCN(C(=O)c2ccc([N+](=O)[O-])cc2)CC1
Mol. weight [g/mol]:	306.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.29		Crippen Method
logp	2.010		Crippen Method
mcvol	224.000	ml/mol	McGowan Method
rinpol	2695.00		NIST Webbook
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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=U361040&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
rinpol:	Non-polar retention indices

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