

Isonipecotic acid, N-(3-methoxybenzoyl)-, pentyl ester

Inchi:	InChI=1S/C19H27NO4/c1-3-4-5-13-24-19(22)15-9-11-20(12-10-15)18(21)16-7-6-8-17(14)
InchiKey:	BRBCHLQZZGHLJU-UHFFFAOYSA-N
Formula:	C19H27NO4
SMILES:	CCCCCOC(=O)C1CCN(C(=O)c2cccc(OC)c2)CC1
Mol. weight [g/mol]:	333.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.02		Crippen Method
logp	3.281		Crippen Method
mcvol	268.810	ml/mol	McGowan Method
rinsol	2792.00		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=U361176&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
rinsol:	Non-polar retention indices

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