

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

Inchi:	InChI=1S/C16H21NO4/c1-3-21-16(19)12-7-9-17(10-8-12)15(18)13-5-4-6-14(11-13)20-2/
InchiKey:	SQUPRMCJHRVBJC-UHFFFAOYSA-N
Formula:	C16H21NO4
SMILES:	CCOC(=O)C1CCN(C(=O)c2cccc(OC)c2)CC1
Mol. weight [g/mol]:	291.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.76		Crippen Method
logp	2.110		Crippen Method
mcvol	226.540	ml/mol	McGowan Method
rinpola	2481.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361172&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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