

Isonipecotic acid, N-(2-methoxybenzoyl)-, octyl ester

Inchi:	InChI=1S/C22H33NO4/c1-3-4-5-6-7-10-17-27-22(25)18-13-15-23(16-14-18)21(24)19-11
InchiKey:	ASYQXDUYEFLFEQ-UHFFFAOYSA-N
Formula:	C22H33NO4
SMILES:	CCCCCCCCOC(=O)C1CCN(C(=O)c2ccccc2OC)CC1
Mol. weight [g/mol]:	375.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.27		Crippen Method
logp	4.451		Crippen Method
mcvol	311.080	ml/mol	McGowan Method
rinpola	3026.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361192&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
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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