

Isonipecotic acid, N-(3-methylbenzoyl)-, tridecyl ester

Inchi:	InChI=1S/C27H43NO3/c1-3-4-5-6-7-8-9-10-11-12-13-21-31-27(30)24-17-19-28(20-18-24
InchiKey:	VJBCBZFWHWKYRI-UHFFFAOYSA-N
Formula:	C27H43NO3
SMILES:	CCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(C)c2)CC1
Mol. weight [g/mol]:	429.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.72		Crippen Method
logp	6.701		Crippen Method
mcvol	375.660	ml/mol	McGowan Method
rinpola	3528.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361108&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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