

Isonipecotic acid, N-(4-methylbenzoyl)-, isoheptyl ester

Inchi:	InChI=1S/C20H29NO3/c1-15(2)5-4-14-24-20(23)18-10-12-21(13-11-18)19(22)17-8-6-16
InchiKey:	MNMKYAKLRUPQLX-UHFFFAOYSA-N
Formula:	C20H29NO3
SMILES:	<chem>Cc1ccc(C(=O)N2CCC(C(=O)OCCCC(C)C)CC2)cc1</chem>
Mol. weight [g/mol]:	331.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.55		Crippen Method
logp	3.827		Crippen Method
mcvol	277.030	ml/mol	McGowan Method
rinpol	2744.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361117&Units=SI

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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