

Isonipecotic acid, N-(4-butylbenzoyl)-, isohexyl ester

Inchi:	InChI=1S/C23H35NO3/c1-4-5-8-19-9-11-20(12-10-19)22(25)24-15-13-21(14-16-24)23(20)
InchiKey:	KYKLTCCROSYIJR-UHFFFAOYSA-N
Formula:	C23H35NO3
SMILES:	CCCCc1ccc(C(=O)N2CCC(C(=O)OCCCC(C)C)CC2)cc1
Mol. weight [g/mol]:	373.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.72		Crippen Method
logp	4.861		Crippen Method
mcvol	319.300	ml/mol	McGowan Method
rinpol	3069.00		NIST Webbook
rinpol	3069.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361132&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
rinpol:	Non-polar retention indices

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