

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

Inchi:	InChI=1S/C22H33NO3/c1-3-5-7-17-26-22(25)20-13-15-23(16-14-20)21(24)19-11-9-18(10)
InchiKey:	YTMRWPFDSVIEIW-UHFFFAOYSA-N
Formula:	C22H33NO3
SMILES:	CCCCCOC(=O)C1CCN(C(=O)c2ccc(CCCC)cc2)CC1
Mol. weight [g/mol]:	359.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.54		Crippen Method
logp	4.615		Crippen Method
mcvol	305.210	ml/mol	McGowan Method
rinpol	3006.00		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=U361131&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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