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

Inchi: InChI=1S/C20H29NO3/c1-3-5-6-16-7-9-17(10-8-16)19(22)21-13-11-18(12-14-21)20(23)2
InchiKey: APGOGCKQLDPVDT-UHFFFAOYSA-N
Formula: C20H29NO3
SMILES: CCCCc1ccc(C(=O)N2CCC(C(=O)OCCC)CC2)cc1
Mol. weight [g/mol]: 331.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.70		Crippen Method
logp	3.835		Crippen Method
mcvol	277.030	ml/mol	McGowan Method
rinpol	2768.00		NIST Webbook
rinpol	2768.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361128&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
rinpol: Non-polar retention indices

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