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

Inchi: InChI=1S/C19H27NO3/c1-3-5-6-15-7-9-16(10-8-15)18(21)20-13-11-17(12-14-20)19(22)2

InchiKey: SSTYJBRTGNVXQT-UHFFFAOYSA-N

Formula: C19H27NO3

SMILES: CCCCc1ccc(C(=O)N2CCC(C(=O)OCC)CC2)cc1

Mol. weight [g/mol]: 317.42

Physical Properties

Property code	Value	Unit	Source
logp	3.444		Crippen Method
mcvol	262.940	ml/mol	McGowan Method
rinpol	2669.00		NIST Webbook
rinpol	2669.00		NIST Webbook
tb	669.45	K	Cheméo Relay (1.0)
tf	319.61	K	Cheméo Relay (1.0)

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361127&Units=SI

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point

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