Isonipecotic acid, N-(4-ethylbenzoyl)-, isobutyl ester

Inchi: InChI=1S/C19H27NO3/c1-4-15-5-7-16(8-6-15)18(21)20-11-9-17(10-12-20)19(22)23-13-1

InchiKey: AMPSRHITULVXNY-UHFFFAOYSA-N

Formula: C19H27NO3

SMILES: CCc1ccc(C(=O)N2CCC(C(=O)OCC(C)C)CC2)cc1

Mol. weight [g/mol]: 317.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.04		Crippen Method
logp	3.300		Crippen Method
mcvol	262.940	ml/mol	McGowan Method
rinpol	2625.00		NIST Webbook
rinpol	2625.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361139&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.