

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

Inchi:	InChI=1S/C19H27NO3/c1-3-5-14-23-19(22)17-10-12-20(13-11-17)18(21)16-8-6-15(4-2)7
InchiKey:	DXJJSTRFYFWGQF-UHFFFAOYSA-N
Formula:	C19H27NO3
SMILES:	CCCCOC(=O)C1CCN(C(=O)c2ccc(CC)cc2)CC1
Mol. weight [g/mol]:	317.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.28		Crippen Method
logp	3.444		Crippen Method
mcvol	262.940	ml/mol	McGowan Method
rinsol	2674.00		NIST Webbook
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Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361140&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinsol:	Non-polar retention indices

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