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

Inchi: InChI=1S/C16H21NO3/c1-3-20-16(19)14-8-10-17(11-9-14)15(18)13-6-4-12(2)5-7-13/h4-
InchiKey: KMGFOPNOABPXRV-UHFFFAOYSA-N
Formula: C16H21NO3
SMILES: CCOC(=O)C1CCN(C(=O)c2ccc(C)cc2)CC1
Mol. weight [g/mol]: 275.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	2.410		Crippen Method
mcvol	220.670	ml/mol	McGowan Method
rinpol	2362.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361112&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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