

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

Inchi: InChI=1S/C23H35NO3/c1-3-5-7-8-18-27-23(26)21-14-16-24(17-15-21)22(25)20-12-10-19
InchiKey: ARUHHGWRXXSMAM-UHFFFAOYSA-N
Formula: C23H35NO3
SMILES: CCCCCOC(=O)C1CCN(C(=O)c2ccc(CCCC)cc2)CC1
Mol. weight [g/mol]: 373.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.96		Crippen Method
logp	5.005		Crippen Method
mcvol	319.300	ml/mol	McGowan Method
rinpol	3113.00		NIST Webbook
rinpol	3113.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.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=U361133&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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