

Isonipecotic acid, N-(3-bromobenzoyl)-, octyl ester

Inchi: InChI=1S/C21H30BrNO3/c1-2-3-4-5-6-7-15-26-21(25)17-11-13-23(14-12-17)20(24)18-9-
InchiKey: XSRYOJMRGPNP-UHFFFAOYSA-N
Formula: C21H30BrNO3
SMILES: CCCCCCOC(=O)C1CCN(C(=O)c2cccc(Br)c2)CC1
Mol. weight [g/mol]: 424.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.32		Crippen Method
logp	5.205		Crippen Method
mcvol	308.620	ml/mol	McGowan Method
rinsol	3179.00		NIST Webbook
rinsol	3179.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361516&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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