

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

Inchi:	InChI=1S/C19H26BrNO3/c1-14(2)5-4-12-24-19(23)15-8-10-21(11-9-15)18(22)16-6-3-7-1
InchiKey:	ONNAFQCKHHGENH-UHFFFAOYSA-N
Formula:	C19H26BrNO3
SMILES:	CC(C)CCCOC(=O)C1CCN(C(=O)c2cccc(Br)c2)CC1
Mol. weight [g/mol]:	396.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.24		Crippen Method
logp	4.281		Crippen Method
mcvol	280.440	ml/mol	McGowan Method
rinpol	2914.00		NIST Webbook
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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=U361513&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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