

Isonipectic acid, N-(3-bromobenzoyl)-, hexyl ester

Inchi:	InChI=1S/C19H26BrNO3/c1-2-3-4-5-13-24-19(23)15-9-11-21(12-10-15)18(22)16-7-6-8-1
InchiKey:	DKCXEGFMXQANSH-UHFFFAOYSA-N
Formula:	C19H26BrNO3
SMILES:	CCCCCOC(=O)C1CCN(C(=O)c2cccc(Br)c2)CC1
Mol. weight [g/mol]:	396.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.48		Crippen Method
logp	4.425		Crippen Method
mcvol	280.440	ml/mol	McGowan Method
rinpol	2967.00		NIST Webbook
rinpol	2967.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361514&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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