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Typical Product Specifications & Properties

1-benzyl-3-bromopyridiniumbromide-B28458

CAS Number: : 928828-19-7

Specifications	Limits
Molecular Formula	C12H11Br2N
Molecular weight	
Canonicalized Compound	1
Compound Complexity	166
Hydrogen Bond Acceptor Count	1
Hydrogen Bond Donor Count	
Rotatable Bond Count	2
Allowed IUPAC Name	1-benzyl-3-bromo-pyridin-1-ium;bromide
CAS-like Style IUPAC Name	3-bromo-1-(phenylmethyl)pyridin-1-ium;bromide
Markup IUPAC Name	1-benzyl-3-bromopyridin-1-ium;bromide
Preferred IUPAC Name	1-benzyl-3-bromopyridin-1-ium;bromide
Systematic IUPAC Name	3-bromanyl-1-(phenylmethyl)pyridin-1-ium;bromide



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Specifications	Limits
Traditional IUPAC Name	1-benzyl-3-bromo-pyridin-1-ium;bromide
Standard InChI	InChI=1S/C12H11BrN.BrH/c13-12-7-4-8-14(10-12)9-11-5-2-1-3-6-11;/h1-8,10H,9H2;1H/q+1;/p-1
Standard InChIKey	FMBNHPKQBARDEZ-UHFFFAOYSA-M
Exact Mass	328.92378
Molecular Weight	329.03
Canonical SMILES	<chem>C1=CC=C(C=C1)C[N+]2=CC=CC(=C2)Br.[Br-]</chem>
Isomeric SMILES	<chem>C1=CC=C(C=C1)C[N+]2=CC=CC(=C2)Br.[Br-]</chem>
Polar Surface Area Topological	3.9
Monoisotopic Weight	326.92582
Chemical Structure	 chemicalStructure-1-benzyl-3-bromopyridiniumbromide-b28458



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