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Typical Product Specifications & Properties

(8a,9R)-9-hydroxy-6'-methoxycinchonanum nicotinate

CAS Number: : 94107-85-4

Specifications	Limits
Molecular weight	447.53
EINECS	302-321-4
SMILES	<chem>N12C(C(c3c4c([n+]cc3)ccc(c4)OC)O)CC(C(C1)C=C)CC2.C(c1cnccc1)[O-]</chem>
InChI	JLKLNKWCCCKPIOP-UHFFFAOYSA-N
InChIKey	1S/C20H24N2O2.C6H5NO2/c1-3-13-12-22-9-7-14(13)10-19(22)20(23)16-6-8-21-18-5-4-15(24-2)11-17(16)18;8-6(9)5-2-1-3-5/h3-6,8,11,13-14,19-20,23H,1,7,9-10,12H2,2H3;1-4H,(H,8,9)



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