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Typical Product Specifications & Properties

(8a,9R)-6'-methoxycinchonan-9-ol, salt with citric acid

CAS Number: : 5936-12-9

Specifications	Limits
Molecular weight	516.54
SMILES	<chem>COc1ccc2c(c1)c(ccn2)[C@H]([C@@H]3CC4CCN3CC4C=C)O.C(C(=O)O)C(CC(=O)O)(C(=O)O)O</chem>
InChI	UTYDQRYLTPTQGW-XCURWTCDSA-N
InChIKey	1S/C20H24N2O2.C6H8O7/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;7-3(8)1-6(13,5(11)12)2-4(9)10/h3-6,8,11,13-14,19-20,23H,1,7,9-10,12H2,2H3;13H,1-2H2,(H,7,8)(H,9,10)(H,11,12)/t13?,14?,19-,20+;/m0./s1



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