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Typical Product Specifications & Properties

Cinchonan-9-ol, 6'-methoxy-, (9S)-, sulfate (2:1)

CAS Number: : 50-54-4

Specifications	Limits
Molecular weight	746.91
EINECS	200-046-3
SMILES	<chem>COc1ccc2c(c1)c(ccn2)[C@@H]([C@H]3C[C@@H]4CC[N@]3C[C@@H]4C=C)O.COc1ccc2c(c1)[C@@H]([C@H]3C[C@@H]4CC[N@]3C[C@@H]4C=C)O.OS(=O)</chem>
InChI	RONWGALEIBILOG-VCSAERELSA-N
InChIKey	1S/2C20H24N2O2.H2O4S/c2*1-3-13-12-22-9-7-14(13)10-19(22)2-6-8-21-18-5-4-15(24-2)11-17(16)18;1-5(2,3)4/h2*3-6,8,11,13-14,120,23H,1,7,9-10,12H2,2H3;(H2,1,2,3,4)/t2*13-,14-,19+,20-;/m00./
pKa Dissociation Constant	4.2
log P (octanol- water)	5.400
Water solubility	1.05E+04 mg/L
Vapor Pressure	3.55E-28 mm Hg
Atmospheric OH Rate Constant	3.70E-10 cm ³ /molecule-sec

