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Typical Product Specifications & Properties

Quinine Hydrobromide

CAS Number: : 549-49-5

Specifications	Limits
Molecular weight	405.33
EINECS	208-967-2
SMILES	<chem>COc1ccc2c(c1)c(ccn2)[C@H]([C@@H]3C[C@@H]4CC[N@]3C[C@@H]4C=C)O.Br</chem>
InChI	HDZGBIRSORQVNB-DSXUQNDKSA-N
InChIKey	1S/C20H24N2O2.BrH/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;/h3-6,8,11,13-14,19-20,23H,1,7,9-10,12H2,2H3;1H/t13-,14-,19-,20+;/m0./s1
Atmospheric OH Rate Constant	1.69E-10 cm ³ /molecule-sec
log P (octanol-water)	1.780
Vapor Pressure	2.08E-17 mm Hg
Henry's Law Constant	4.30E-23 atm-m ³ /mole
Water solubility	2.33E+04 mg/L



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