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Typical Product Specifications & Properties

(1S)-(6-Methoxyquinolin-4-yl) ((2R,4S,5R)-5-vinylquinuclidin-2-yl)methanol

CAS Number: : 56-54-2

Specifications	Limits
Molecular weight	324.42
SMILES	<chem>COc1ccc2nccc([C@H](O)[C@H]3C[C@@H]4CCN3C[C@@H]4C=C)c2c1</chem>
InChI	1S/C20H24N2O2/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/t13?,14?,19?,20-/m1/s1
InChIKey	LOUPRKONTZGTKE-WGFDLZGGSA-N
Vapor Pressure	1.10E-10 mm Hg
Melting Point	174 ° C
log P (octanol-water)	3.44
pKa Dissociation Constant	8.56
Henry's Law Constant	8.58E-16 atm-m ³ /mole
Water solubility	140 mg/L
Atmospheric OH Rate Constant	1.75E-10 cm ³ /molecule-sec

ISO 9001



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