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Typical Product Specifications & Properties

(8a)-6'-methoxycinchonan-9-one

CAS Number: : 84-31-1

Specifications	Limits
Molecular weight	322.40
EINECS	201-524-4
SMILES	<chem>COc1ccc2c(c1)c(ccn2)C(=O)[C@@H]3C[C@@H]4CC[N@]3C[C@@H]4C=C</chem>
InChI	SRFCUPVBYYAMIL-NJSLBKSFSA-N
InChIKey	1S/C20H22N2O2/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/h3-6,8,11,13-14,19H,1,7,9-10,12H2,2H3/t13-,14-,19-/m0/s1
Atmospheric OH Rate Constant	1.11E-10 cm ³ /molecule-sec
Melting Point	108 ° C
log P (octanol-water)	4.240
Water solubility	3 mg/L



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415 Huguenot Street, New Rochelle, New York 10801

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