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Typical Product Specifications & Properties

Demecycline

CAS Number: : 987-02-0

Specifications	Limits
Molecular weight	430.41
SMILES	<chem>CN(C)[C@H]1[C@@H]2C[C@@H]3[C@@H](c4cccc(c4C(=O)C3=C([C@@]2(C(=O)C(=C1O)C(=O)N)O)C</chem>
InChI	JCSGAUKCDAVARS-SOUFLCLCSA-N
InChIKey	1S/C21H22N2O8/c1-23(2)14-9-6-8-12(16(26)11-7(15(8)25)4-3-5-10(11)24)18(28)21(9,31)19(29)13(17(14)27)20(22)30/h3-5,8-9,15,24-25,27-28,31H,6H2,1-2H3,(H2,22,30)/t8-,9-,14-,15+,21-/m0/s



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