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Typical Product Specifications & Properties

Semixylenol Orange

CAS Number: : 19329-67-0

Specifications	Limits
Molecular weight	527.54
SMILES	<chem>C(CN(Cc1c(c(cc(c1)[C@@]1(OS(c2c1cccc2)(=O)=O)c1cc(c(cc1)O)C)C)O)CC(=O)O)(=O)O</chem>
InChI	OGODTFKKGYRAQJ-UHFFFAOYSA-N
InChIKey	1S/C26H25NO9S/c1-15-9-18(7-8-21(15)28)26(20-5-3-4-6-22(20)37(34,35)36-26)19-10-16(2)25(33)17(11-19)12-27(13-23(29)30)14-24(31)32/h3-11,28,33H,12-14H2,1-2H3,(H,29,30)(H,31,32)
Chemical Structure	 140381_140381_semixylenol-orange.png chemical structure



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