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Typical Product Specifications & Properties

Xylenol Orange

CAS Number: : 1611-35-4

Specifications	Limits
Molecular weight	672.66
EINECS	216-553-8
SMILES	<chem>S1(OC(c2cc(CN(CC(=O)O)CC(=O)O)c(c(c2)C)O)(c2cc(CN(CC(=O)O)CC(=O)O)c(c(c2)C)O)c2c1cccc2)(=O)=O</chem>
InChI	ORZHVITYKPFVVMG-UHFFFAOYSA-N
InChIKey	1S/C31H32N2O13S/c1-17-7-21(9-19(29(17)42)11-32(13-25(34)35)14-26(36)37)31(23-5-3-4-6-24(23)47(44,45)46-31)22-8-18(2)30(43)20(10-22)12-33(15-27(38)39)16-28(40)41/h3-10,42-43H,11-16H2,1-2H3,(H,34,35)(H,36,37)(H,38,39)(H,40,41)
Chemical Structure	 89376 89376_xylenol-orange.png chemical structure



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