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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            | ORZHVTYKPFVVMG-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) |



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