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## Typical Product Specifications & Properties

### Isoxyl

CAS Number: : 910-86-1

| Specifications               | Limits                                                                                                                                    |
|------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Molecular weight             | 400.58                                                                                                                                    |
| EINECS                       | 213-006-5                                                                                                                                 |
| SMILES                       | <chem>c1(NC(Nc2ccc(OCCC(C)C)cc2)=S)ccc(OCCC(C)C)cc1</chem>                                                                                |
| InChI                        | 1S/C23H32N2O2S/c1-17(2)13-15-26-21-9-5-19(6-10-21)24-23(28)25-20-7-11-22(12-8-20)27-16-14-18(3)4/h5-12,17-18H,13-16H2,1-4H3,(H2,24,25,28) |
| InChIKey                     | BWBONKHPVHMQHE-UHFFFAOYSA-N                                                                                                               |
| log P (octanol-water)        | 7.160                                                                                                                                     |
| Melting Point                | 146 &deg; C                                                                                                                               |
| Atmospheric OH Rate Constant | 1.01E-10 cm <sup>3</sup> /molecule-sec                                                                                                    |



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