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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/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 ° C |
| Atmospheric OH Rate Constant | 1.01E-10 cm ³ /molecule-sec |



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