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

