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Typical Product Specifications & Properties

C.I. 13020

CAS Number: : 493-52-7

| Specifications | Limits |
|------------------------------|--|
| Molecular weight | 269.30 |
| EINECS | 207-776-1 |
| SMILES | <chem>c1(c(ccc1)C(O)=O)\N=N\c1ccc(N(C)C)cc1</chem> |
| InChI | 1S/C15H15N3O2/c1-18(2)12-9-7-11(8-10-12)16-17-14-6-4-3-5-13(14)15(19)20/h3-10H,1-2H3,(H,19,20) |
| InChIKey | CEQFOVLGLXCDCX-UHFFFAOYSA-N |
| pKa Dissociation Constant | 2.63 |
| Henry's Law Constant | 4.71E-12 atm-m ³ /mole |
| Vapor Pressure | 1.44E-07 mm Hg |
| Atmospheric OH Rate Constant | 1.50E-10 cm ³ /molecule-sec |
| log P (octanol-water) | 3.830 |
| Melting Point | 183 ° C |
| Water solubility | 3.670 mg/L |



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