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Typical Product Specifications & Properties

Sulphamethazine Sodium Salt

CAS Number: : 1981-58-4


| Specifications | Limits |
|----------------------|---|
| Molecular weight | 300.31 |
| EINECS | 217-840-0 |
| SMILES | <chem>Cc1cc(nc(n1)[N-]S(=O)(=O)c2ccc(cc2)N)C.[Na+]</chem> |
| InChI | NGIVTUVVBWOTNT-UHFFFAOYSA-N |
| InChIKey | 1S/C12H13N4O2S.Na/c1-8-7-9(2)15-12(14-8)16-19(17,18)11-5-3-10(13)4-6-11;/h3-7H,13H2,1-2H3;/q-1;+1 |
| Molecular weight | 280.30 |
| EINECS | 201-272-5 |
| SMILES | <chem>c1(S(=O)(=O)Nc2ccc(nn2)OC)ccc(cc1)N</chem> |
| InChI | 1S/C11H12N4O3S/c1-18-11-7-6-10(13-14-11)15-19(16,17)9-4-2-8(12)3-5-9/h2-7H,12H2,1H3,(H,13,15) |
| InChIKey | VLYWMPOKSSWJAL-UHFFFAOYSA-N |
| Henry's Law Constant | 2.37E-14 atm-m ³ /mole |
| Melting Point | 182.5 °C |





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| Specifications | Limits |
|------------------------------|---|
| Water solubility | 147 mg/L |
| log P (octanol-water) | 0.32 |
| Atmospheric OH Rate Constant | 2.82E-11 cm ³ /molecule-sec |
| pKa Dissociation Constant | 6.7 |
| Vapor Pressure | 5.65E-10 mm Hg |
| Storage Temperature | 2-8°C |
| Form | Crystalline Powder |
| Merck | 13,9004 |
| Color | White to yellow |
| Chemical Structure |  88945_88945_sulphamethazine-sodium-salt.png chemical structure |



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