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Typical Product Specifications & Properties

Sulphanilylurea

CAS Number: : 547-44-4

| Specifications | Limits |
|------------------------------|---|
| Molecular weight | 215.23 |
| EINECS | 208-922-7 |
| SMILES | <chem>c1(N)ccc(S(=O)(=O)N)cc1</chem> |
| InChI | 1S/C7H9N3O3S/c8-5-1-3-6(4-2-5)14(12,13)10-7(9)11/h1-4H,8H2,(H3,9,10,11) |
| InChIKey | WVAKABMNNSMCDK-UHFFFAOYSA-N |
| Water solubility | 1200 mg/L |
| Atmospheric OH Rate Constant | 2.50E-11 cm ³ /molecule-sec |
| Melting Point | 147 dec ° C |
| log P (octanol-water) | -1.000 |
| Molecular weight | 214.25 |
| EINECS | 200-345-9 |
| SMILES | <chem>c1cc(ccc1N)S(=O)(=O)NC(=N)N</chem> |



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| Specifications | Limits |
|------------------------------|--|
| InChI | 1S/C7H10N4O2S/c8-5-1-3-6(4-2-5)14(12,13)11-7(9)10/h1-4H,8H2,(H4,9,10,11) |
| InChIKey | BRBKOPJOKNSWSG-UHFFFAOYSA-N |
| Atmospheric OH Rate Constant | 4.40E-11 cm ³ /molecule-sec |
| pKa Dissociation Constant | 11.25 |
| Vapor Pressure | 1.47E-07 mm Hg |
| Melting Point | 191.5 ° C |
| Water solubility | 2200 mg/L |
| log P (octanol-water) | -1.22E+00 |
| Henry's Law Constant | 1.01E-15 atm-m ³ /mole |
| Solubility | 1 M HCl: soluble50mg/mL |
| Merck | 8908 |
| Stability | Stable. Incompatible with strong oxidizing agents. |



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| Specifications | Limits |
|---------------------|--------------------|
| Water solubility | 1g/1000mL at 25 °C |
| Melting Point | 190-193°C |
| Storage Temperature | -20°C |
| Color | white to off-white |
| Form | Powder |



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