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## Typical Product Specifications & Properties

# Pyrazine-N-Oxide

CAS Number: : 2423-65-6

| Specifications   | Limits                                                                                                                                                |
|------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------|
| Molecular weight | 96.09                                                                                                                                                 |
| SMILES           | <chem>n1(=O)ccncc1</chem>                                                                                                                             |
| InChI            | RUIZBQQGWNBRFH-UHFFFAOYSA-N                                                                                                                           |
| InChIKey         | 1S/C4H4N2O/c7-6-3-1-5-2-4-6/h1-4H                                                                                                                     |
| Molecular weight | 623.49                                                                                                                                                |
| EINECS           | 222-530-3                                                                                                                                             |
| SMILES           | <chem>Cc1nn(c(O)c1N=Nc2ccc(cc2Cl)c3ccc(N=Nc4c(C)nn(c4O)c4ccccc4)cc3)cc1</chem>                                                                        |
| InChI            | LVOJOIBIVGEQBP-ATXIYDNESA-N                                                                                                                           |
| InChIKey         | 1S/C32H24Cl2N8O2/c1-19-29(31(43)41(39-19)23-9-5-3-6-10-23).25(27)33)22-14-16-28(26(34)18-22)36-38-30-20(2)40-42(32(30)418,43-44H,1-2H3/b37-35+,38-36+ |
| Colour Index     | 21110                                                                                                                                                 |



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