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## Typical Product Specifications & Properties

# Clozapine

CAS Number: : 5786-21-0

| Specifications               | Limits                                                                                                        |
|------------------------------|---------------------------------------------------------------------------------------------------------------|
| Molecular weight             | 326.82                                                                                                        |
| SMILES                       | <chem>CN1CCN(CC1)C2=Nc3cc(ccc3Nc4c2cccc4)Cl</chem>                                                            |
| InChI                        | 1S/C18H19ClN4/c1-22-8-10-23(11-9-22)18-14-4-2-3-5-15(14)20-16-7-6-13(19)12-17(16)21-18/h2-7,12,20H,8-11H2,1H3 |
| InChIKey                     | QZUDBNBUXVUHMW-UHFFFAOYSA-N                                                                                   |
| pKa Dissociation Constant    | 7.5                                                                                                           |
| Atmospheric OH Rate Constant | 3.76E-10 cm <sup>3</sup> /molecule-sec                                                                        |
| Water solubility             | 11.8 mg/L                                                                                                     |
| log P (octanol-water)        | 3.23                                                                                                          |
| Vapor Pressure               | 9.48E-09 mm Hg                                                                                                |
| Henry's Law Constant         | 9.29E-15 atm-m <sup>3</sup> /mole                                                                             |
| Melting Point                | 183-184 &deg; C                                                                                               |



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415 Huguenot Street, New Rochelle, New York 10801

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