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## Typical Product Specifications & Properties

# 1,3,5-Trinitrobenzene

CAS Number: : 99-35-4

| Specifications               | Limits  |
|------------------------------|---|
| Molecular weight             | 213.10  |
| EINECS                       | 202-752-7   |
| SMILES                       | <chem>c1(cc(cc(c1)[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]</chem> |
| InChI                        | 1S/C6H3N3O6/c10-7(11)4-1-5(8(12)13)3-6(2-4)9(14)15/h1-3H        |
| InChIKey                     | UATJOMSPNYCXIX-UHFFFAOYSA-N                                     |
| Boiling Point                | 315 &deg; C   |
| log P (octanol-water)        | 1.18  |
| Atmospheric OH Rate Constant | 1.30E-15 cm <sup>3</sup> /molecule-sec                          |
| Henry's Law Constant         | 3.31E-10 atm-m <sup>3</sup> /mole                               |
| Water solubility             | 278 mg/L  |
| Melting Point                | 121.5 &deg; C   |
| Melting Point                | 122&deg;C   |





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| Specifications      | Limits    |
|---------------------|-----------|
| Storage Temperature | 2-8&deg;C |
| Merck               | 9726      |



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415 Huguenot Street, New Rochelle, New York 10801

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