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## Typical Product Specifications & Properties

# Nitrilotriacetic acid

CAS Number: : 139-13-9

| Specifications               | Limits   |
|------------------------------|--|
| Molecular weight             | 191.14   |
| EINECS                       | 205-355-7  |
| SMILES                       | <chem>N(CC(O)=O)(CC(O)=O)CC(O)=O</chem>                                    |
| InChI                        | 1S/C6H9NO6/c8-4(9)1-7(2-5(10)11)3-6(12)13/h1-3H2,(H,8,9)(H,10,11)(H,12,13) |
| InChIKey                     | MGFYIUFZLHCRTH-UHFFFAOYSA-N  |
| Henry's Law Constant         | 1.30E-10 atm-m <sup>3</sup> /mole  |
| Melting Point                | 242 dec &deg; C  |
| log P (octanol-water)        | -3.810   |
| Atmospheric OH Rate Constant | 7.90E-11 cm <sup>3</sup> /molecule-sec                                     |
| Vapor Pressure               | 7.00E-09 mm Hg   |
| Water solubility             | 5.91E+04 mg/L  |
| pKa Dissociation Constant    | 3.03   |



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| Specifications      | Limits   |
|---------------------|--|
| Melting Point       | 245 &deg;C (dec.)                                |
| Water solubility    | Insoluble.<0.01 g/100 mL at 23 &#186;C           |
| Flash Point         | 100 &deg;C                                       |
| Storage Temperature | Store at room temperature.                       |
| Merck               | 14,6579  |
| Solubility          | 0.1 M NaOH: 0.1 M at 20 &deg;C, clear, colorless |



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