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Typical Product Specifications & Properties

1,3-Dimethyl-2-nitrobenzene

CAS Number: : 81-20-9

| Specifications | Limits |
|------------------------------|---|
| Molecular weight | 151.16 |
| SMILES | <chem>c1(c(ccc1C)C)[N+](=O)[O-]</chem> |
| InChI | 1S/C8H9NO2/c1-6-4-3-5-7(2)8(6)9(10)11/h3-5H,1-2H3 |
| InChIKey | HDFQKJQEWGVKCCQ-UHFFFAOYSA-N |
| Henry's Law Constant | 2.59E-05 atm-m3/mole |
| Melting Point | 15 ° C |
| log P (octanol-water) | 2.95 |
| Boiling Point | 226 ° C |
| Vapor Pressure | 0.020 mm Hg |
| Water solubility | 92.4 mg/L |
| Atmospheric OH Rate Constant | 1.93E-12 cm3/molecule-sec |



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