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## Typical Product Specifications & Properties

# 3-Nitrobiphenyl

CAS Number: : 2113-58-8

| Specifications               | Limits                                                       |
|------------------------------|--------------------------------------------------------------|
| Molecular weight             | 199.21                                                       |
| EINECS                       | 218-305-4                                                    |
| SMILES                       | <chem>c1(c2ccccc2)cc(ccc1)[N+](=O)[O-]</chem>                |
| InChI                        | 1S/C12H9NO2/c14-13(15)12-8-4-7-11(9-12)10-5-2-1-3-6-10/h1-9H |
| InChIKey                     | FYRPEHRWMVMHQM-UHFFFAOYSA-N                                  |
| Atmospheric OH Rate Constant | 2.79E-12 cm <sup>3</sup> /molecule-sec                       |
| log P (octanol-water)        | 3.87                                                         |
| Melting Point                | 62 &deg; C                                                   |
| Water solubility             | 1.370 mg/L                                                   |
| Henry's Law Constant         | 1.63E-06 atm-m <sup>3</sup> /mole                            |
| Vapor Pressure               | 3.25E-05 mm Hg                                               |
| BRN Number                   | 1872195                                                      |



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| Specifications | Limits               |
|----------------|----------------------|
| Flash Point    | 227&deg;C/35mm       |
| Melting Point  | 58-60 &deg;C         |
| Boiling Point  | 227 &deg;C (35 mmHg) |



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