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## Typical Product Specifications & Properties

# Dibutyl ether

CAS Number: : 142-96-1

| Specifications      | Limits                                    |
|---------------------|-------------------------------------------|
| Molecular weight    | 130.23                                    |
| EINECS              | 205-575-3                                 |
| InChI               | 1S/C8H18O/c1-3-5-7-9-8-6-4-2/h3-8H2,1-2H3 |
| InChIKey            | DURPTKYDGMDSBL-UHFFFAOYSA-N               |
| BRN Number          | 1732752                                   |
| Vapor Density       | 4.48                                      |
| Merck               | 14,1569                                   |
| Melting Point       | -98 &deg;C                                |
| Refractive Index    | 1.399                                     |
| Boiling Point       | 142-143 &deg;C                            |
| Density             | 0.764 g/mL at 25 &deg;C                   |
| Storage Temperature | Flammables area                           |



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| Specifications   | Limits                                                                                                                 |
|------------------|------------------------------------------------------------------------------------------------------------------------|
| Stability        | Stable. Flammable. May form peroxides in storage. Incompatible with strong oxidizing agents.                           |
| Flash Point      | 77 &deg;F                                                                                                              |
| Water solubility | 0.03 g/100 mL (20 °C)                                                                                                  |
| Vapor Pressure   | 4.8 mm Hg ( 20 &deg;C)                                                                                                 |
| Molecular weight | 388.20                                                                                                                 |
| EINECS           | 215-811-7                                                                                                              |
| SMILES           | <chem>c1cc(c(cc1[N+](=O)[O-])Cl)NC(=O)c2cc(ccc2O)Cl.C(CO)N</chem>                                                      |
| InChI            | XYCDHXSQODHSLG-UHFFFAOYSA-N                                                                                            |
| InChIKey         | 1S/C13H8Cl2N2O4.C2H7NO/c14-7-1-4-12(18)9(5-7)13(19)16-11-3-2-8(17(20)21)6-10(11)15;3-1-2-4/h1-6,18H,(H,16,19);4H,1-3H2 |
| Stability        | Stable. Hydrolyzes in concentrated acidic or basic solutions.                                                          |
| Water solubility | 100 mg/L                                                                                                               |
| Vapor Pressure   | 1.00E-14 mm Hg                                                                                                         |



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| Specifications               | Limits                                 |
|------------------------------|----------------------------------------|
| Melting Point                | 216 &deg; C                            |
| Atmospheric OH Rate Constant | 2.10E-11 cm <sup>3</sup> /molecule-sec |
| log P (octanol-water)        | 0.680                                  |
| Specifications               | Limits                                 |
| Henry's Law Constant         | 4.30E-20 atm-m <sup>3</sup> /mole      |



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