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## Typical Product Specifications & Properties

# 1-benzyl-3-methylimidazolium tetrafluoroborate

CAS Number: : 500996-04-3

| Specifications            | Limits  |
|---------------------------|---|
| Molecular weight          | 260.04  |
| Molecular weight          | 241.29  |
| EINECS                    | 200-513-1   |
| SMILES                    | <chem>c1(c(ccc1)C(=O)O)Nc1c(c(ccc1)C)C</chem>   |
| InChI                     | 1S/C15H15NO2/c1-10-6-5-9-13(11(10)2)16-14-8-4-3-7-12(14)15(17)18/h3-9,16H,1-2H3,(H,17,18) |
| InChIKey                  | HYYBABOKPJLUIN-UHFFFAOYSA-N   |
| Merck                     | 5798  |
| Melting Point             | 230 &deg;C  |
| log P (octanol-water)     | 5.12  |
| pKa Dissociation Constant | 4.2   |
| Water solubility          | 20 mg/L   |
| Vapor Pressure            | 4.63E-07 mm Hg  |



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| Specifications               | Limits   |
|------------------------------|--|
| Melting Point                | 230-231 &deg; C  |
| Henry's Law Constant         | 2.57E-11 atm-m3/mole   |
| Atmospheric OH Rate Constant | 2.01E-10 cm3/molecule-sec  |
| Water solubility             | It is soluble in acetone, chloroform, dichloromethane, methanol. Insoluble in water. |
| Storage Temperature          | Refrigerator   |



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