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Typical Product Specifications & Properties

1,4-Benzenedicarboxylic acid

CAS Number: : 100-21-0

| Specifications | Limits |
|------------------------------|---|
| pKa Dissociation Constant | 3.51 |
| Atmospheric OH Rate Constant | 2.75E-13 cm ³ /molecule-sec |
| Water solubility | 15 mg/L |
| Henry's Law Constant | 3.88E-13 atm-m ³ /mole |
| Melting Point | >300 ° C |
| log P (octanol-water) | 2 |
| Melting Point | 300 °C |
| Water solubility | slightly soluble in water (0.017 g/L at 25°C) |
| BRN Number | 1909333 |
| Vapor Pressure | <0.01 mm Hg (20 °C) |
| Stability | Stable. Combustible. Incompatible with strong oxidizing agents. |
| Merck | 14&9162 |



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| Specifications | Limits |
|---------------------|---|
| Density | 1.51 g/cm ³ |
| Storage Temperature | 0-6°C |
| Flash Point | 260°C |
| EINECS | 202-830-0 |
| Molecular weight | 166.1308 |
| SMILES | <chem>c1(C(O)=O)ccc(C(O)=O)cc1</chem> |
| InChIKey | 1S/C8H6O4/c9-7(10)5-1-2-6(4-3-5)8(11)12/h1-4H&(H&9&10)(H&11&12) |
| InChI | KKEYFWRCBNTPAC-UHFFFAOYSA-N |



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