

## Typical Product Specifications & Properties

# Pyrocatechol

**CAS Number: 120-80-9**

| Specifications               | Limits                                 |
|------------------------------|--|
| Molecular weight             | 110.11                                 |
| SMILES                       | <chem>c1(c(ccc1)O)O</chem>             |
| InChI                        | 1S/C6H6O2/c7-5-3-1-2-4-6(5)8/h1-4,7-8H |
| InChIKey                     | YCIMNLLNPGFGHC-UHFFFAOYSA-N            |
| Boiling Point                | 245 ° C                                |
| Melting Point                | 105 ° C                                |
| Atmospheric OH Rate Constant | 1.04E-10 cm <sup>3</sup> /molecule-sec |
| Henry's Law Constant         | 3.14E-09 atm-m <sup>3</sup> /mole      |
| pKa Dissociation Constant    | 9.45                                   |
| log P (octanol-water)        | 0.88                                   |
| Water solubility             | 4.61E+05 mg/L                          |