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## Typical Product Specifications & Properties

# Methyl vanillate

CAS Number: : 3943-74-6

| Specifications               | Limits   |
|------------------------------|--|
| Molecular weight             | 182.17   |
| SMILES                       | <chem>c1(cc(c(O)cc1)OC)C(OC)=O</chem>                      |
| InChI                        | 1S/C9H10O4/c1-12-8-5-6(9(11)13-2)3-4-7(8)10/h3-5,10H,1-2H3 |
| InChIKey                     | BVWTXUYLKBHMOX-UHFFFAOYSA-N                                |
| Atmospheric OH Rate Constant | 1.04E-11 cm <sup>3</sup> /molecule-sec                     |
| Boiling Point                | 286 &deg; C  |
| Melting Point                | 64 &deg; C   |
| log P (octanol-water)        | 1.820  |



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