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## Typical Product Specifications & Properties

# Benzoylacetone

CAS Number: : 93-91-4

| Specifications               | Limits                                                  |
|------------------------------|---------------------------------------------------------|
| Molecular weight             | 162.19                                                  |
| SMILES                       | <chem>c1(C(CC(C)=O)=O)ccccc1</chem>                     |
| InChI                        | 1S/C10H10O2/c1-8(11)7-10(12)9-5-3-2-4-6-9/h2-6H,7H2,1H3 |
| InChIKey                     | CVBUKMMMRLOKQR-UHFFFAOYSA-N                             |
| Atmospheric OH Rate Constant | 2.40E-12 cm <sup>3</sup> /molecule-sec                  |
| Boiling Point                | 261.5 &deg; C                                           |
| log P (octanol-water)        | 0.610                                                   |
| Water solubility             | 383 mg/L                                                |
| Melting Point                | 56 &deg; C                                              |



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