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## Typical Product Specifications & Properties

# 11 $\beta$ ,17,21-trihydroypregn-4-ene-3,20-dione 21-(3,3-dimethylbutyrate)

CAS Number: : 508-96-3

| Specifications               | Limits   |
|------------------------------|--|
| Molecular weight             | 460.60   |
| EINECS                       | 208-090-5  |
| SMILES                       | <chem>C[C@]12CCC(=O)C=C1CC[C@@H]3[C@@H]2[C@H](C[C@]4([C@H]3CC[C@@]4(C(=O)COC(=O)CC(C)(C)C)O)C)O</chem>   |
| InChI                        | FNFPHNZQOKBKHN-KAJVQRHSA-N   |
| InChIKey                     | 1S/C27H40O6/c1-24(2,3)14-22(31)33-15-21(30)27(32)11-9-19-18-7-6-16-12-17(28)8-10-25(16,4)23(18)20(29)13-26(19,27)5/h12,18-20,23,29,32H,6-11,13-15H2,1-5H3/t18-,19-,20-,23+,25-,26-,27-/m0/s1 |
| Atmospheric OH Rate Constant | 1.14E-10 cm <sup>3</sup> /molecule-sec   |
| log P (octanol-water)        | 4.210  |
| Melting Point                | 168 &deg; C  |
| Water solubility             | 1.42 mg/L  |



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