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## Typical Product Specifications & Properties

# 4-alpha,8-alpha,9-beta,11-alpha,13-alpha,14-beta,16-beta,17z)-ph

CAS Number: : 6990-06-3

| Specifications                     | Limits                                                                                                                                                                                                                                |
|------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Molecular weight                   | 516.71                                                                                                                                                                                                                                |
| EINECS                             | 230-256-0                                                                                                                                                                                                                             |
| SMILES                             | <chem>C1[C@@]2([C@@]3([C@H](\C(=C(/CC\C=C(/C)C)C(O)=O)[C@H](C3)OC(C)=O)[C@H]([C@@H]2[C@@]2([C@@H]([C@@H]([C@H](O)CC2)C)C1)C)O)C)C</chem>                                                                                              |
| InChI                              | IECPWNUMDGFDKC-MZJAQBGESA-N                                                                                                                                                                                                           |
| InChIKey                           | 1S/C31H48O6/c1-17(2)9-8-10-20(28(35)36)26-22-15-24(34)27-29(5)13-12-23(33)18(3)21(29)11-14-30(27,6)31(22,7)16-25(26)37-19(4)32/h9,18,21-25,27,33-34H,8,10-16H2,1-7H3,(H,35,36)/b26-20-/t18-,21-,22-,23+,24+,25-,27-,29-,30-,31-/m0/s1 |
| Melting Point                      | 192.5 &deg; C                                                                                                                                                                                                                         |
| log P (octanol-water)              | 6.750                                                                                                                                                                                                                                 |
| pKa<br>Dissociation<br>Constant    | 5.35                                                                                                                                                                                                                                  |
| Atmospheric<br>OH Rate<br>Constant | 1.72E-10 cm <sup>3</sup> /molecule-sec                                                                                                                                                                                                |

ISO 9001



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