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Typical Product Specifications & Properties

17-B-Estradiol Benzoate

CAS Number: : 50-50-0

| Specifications | Limits |
|------------------------------|--|
| Molecular weight | 376.49 |
| EINECS | 200-043-7 |
| SMILES | <chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(OC(=O)c5ccccc5)ccc34)[C@@H]1CC[C@H]2O</chem> |
| InChI | 1S/C25H28O3/c1-25-14-13-20-19-10-8-18(28-24(27)16-5-3-2-4-6-16)15-17(19)7-9-21(20)22(25)11-12-23(25)26/h2-6,8,10,15,20-23,26H,7,9,11-14H2,1H3/t20-,21-,22+,23+,25+/m0/s1 |
| InChIKey | UYIFTLBWAOGQBI-PPWDSJTCSA-N |
| Melting Point | 196 ° C |
| log P (octanol-water) | 5.470 |
| Atmospheric OH Rate Constant | 3.07E-11 cm ³ /molecule-sec |
| Melting Point | 191-198 °C |
| Merck | 3703 |



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