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Typical Product Specifications & Properties

Pravastatin Lactone

CAS Number: : 85956-22-5

| Specifications | Limits |
|------------------------------|---|
| SMILES | <chem>CC[C@H](C)C(=O)O[C@H]1C[C@H](O)C=C2C=C[C@H](C)[C@H](CC[C@@H]3C[C@@H](O)CC(=O)O3)[C@@H]12</chem> |
| InChI | OQARDMYXSOFTLN-PZ AWKZ KUSA-N |
| InChIKey | 1S/C23H34O6/c1-4-13(2)23(27)29-20-11-16(24)9-15-6-5-14(3)19(22(15)20)8-7-18-10-17(25)12-21(26)28-18/h5-6,9,13-14,16-20,22,24-25H,4,7-8,10-12H2,1-3H3/t13-,14-,16+,17+,18+,19-,20-,22-/m0/s1 |
| log P (octanol-water) | 2.42 |
| Water solubility | 23.9 mg/L |
| Henry's Law Constant | 5.84E-12 atm-m ³ /mole |
| Vapor Pressure | 2.82E-14 mm Hg |
| Atmospheric OH Rate Constant | 2.36E-10 cm ³ /molecule-sec |



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