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## Typical Product Specifications & Properties

# (±)-2-Hydroxy-2-phenylpropionic acid hemihydrate

CAS Number: : 515-30-0

| Specifications               | Limits  |
|------------------------------|---|
| Molecular weight             | 166.17  |
| SMILES                       | <chem>c1([C@@](C(O)=O)(C)O)ccccc1</chem>                        |
| InChI                        | 1S/C9H10O3/c1-9(12,8(10)11)7-5-3-2-4-6-7/h2-6,12H,1H3,(H,10,11) |
| InChIKey                     | NWCHELUCVWSRRS-UHFFFAOYSA-N                                     |
| Water solubility             | 2.12E+04 mg/L   |
| log P (octanol-water)        | 0.8   |
| Atmospheric OH Rate Constant | 5.47E-12 cm <sup>3</sup> /molecule-sec                          |
| Melting Point                | 116.5 &deg; C   |
| Henry's Law Constant         | 9.16E-09 atm-m <sup>3</sup> /mole                               |
| Vapor Pressure               | 1.39E-05 mm Hg  |
| pKa Dissociation Constant    | 3.53  |

