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## Typical Product Specifications & Properties

# Bis(6-methylheptyl) phthalate

CAS Number: : 27554-26-3

| Specifications               | Limits                                                                                                                                |
|------------------------------|---------------------------------------------------------------------------------------------------------------------------------------|
| Molecular weight             | 390.56                                                                                                                                |
| EINECS                       | 248-523-5                                                                                                                             |
| SMILES                       | <chem>CC(C)CCCCCOC(=O)c1ccccc1C(=O)OCCCCC(C)C</chem>                                                                                  |
| InChI                        | IJFPVINAQGWB RJ-UHFFFAOYSA-N                                                                                                          |
| InChIKey                     | 1S/C24H38O4/c1-19(2)13-7-5-11-17-27-23(25)21-15-9-10-16-22(21)24(26)28-18-12-6-8-14-20(3)4/h9-10,15-16,19-20H,5-8,11-14,17-18H2,1-4H3 |
| Henry's Law Constant         | 3.14E-05 atm-m <sup>3</sup> /mole                                                                                                     |
| Atmospheric OH Rate Constant | 2.06E-11 cm <sup>3</sup> /molecule-sec                                                                                                |
| log P (octanol-water)        | 8.390                                                                                                                                 |
| Water solubility             | 0.09 mg/L                                                                                                                             |
| Vapor Pressure               | 5.50E-06 mm Hg                                                                                                                        |
| Boiling Point                | 235 &deg; C                                                                                                                           |
| Melting Point                | -5.00E+01 &deg; C                                                                                                                     |



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| Specifications   | Limits                  |
|------------------|-------------------------|
| Refractive Index | 1.486                   |
| Density          | 0.983 g/mL at 25 &deg;C |
| Vapor Pressure   | 1 mm Hg ( 200 &deg;C)   |
| Flash Point      | >230 &deg;F             |



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