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Typical Product Specifications & Properties

2,3-dihydro-3,3-dimethyl-5-benzofurylethanesulphonate

CAS Number: : 68505-69-1

| Specifications | Limits |
|------------------------------|--|
| Molecular weight | 256.32 |
| EINECS | 270-925-4 |
| SMILES | <chem>CCS(=O)(=O)Oc1ccc2c(c1)C(CO2)(C)C</chem> |
| InChI | QGQSRQPXXMTJCM-UHFFFAOYSA-N |
| InChIKey | 1S/C12H16O4S/c1-4-17(13,14)16-9-5-6-11-10(7-9)12(2,3)8-15-11/h5-7H,4,8H2,1-3H3 |
| Water solubility | 261 mg/L |
| log P (octanol-water) | 2.41 |
| Atmospheric OH Rate Constant | 1.12E-11 cm ³ /molecule-sec |
| Vapor Pressure | 2.09E-05 mm Hg |
| Henry's Law Constant | 2.70E-08 atm-m ³ /mole |
| Melting Point | 30.1 °C |

