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Typical Product Specifications & Properties

4-n-Octylbenzoic acid

CAS Number: : 3575-31-3

| Specifications | Limits |
|------------------|--|
| Molecular weight | 234.33 |
| EINECS | 222-692-5 |
| SMILES | <chem>c1(ccc(C(=O)=O)cc1)CCCCCCCC</chem> |
| InChI | ZQLDNJKHLQOJGE-UHFFFAOYSA-N |
| InChIKey | 1S/C15H22O2/c1-2-3-4-5-6-7-8-13-9-11-14(12-10-13)15(16)17/h9-12H,2-8H2,1H3,(H,16,17) |
| Density | 1.002 |
| BRN Number | 1954607 |
| Water solubility | Soluble in methanol, hot hexane, hot ethanol and 2-propanol and toluene. Insoluble in water. |
| Melting Point | 97-98 °C |



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