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## Typical Product Specifications & Properties

# Isethionic Acid, Free Base

CAS Number: : 107-36-8

| Specifications               | Limits  |
|------------------------------|---|
| Molecular weight             | 126.13  |
| EINECS                       | 203-484-3                                     |
| SMILES                       | <chem>OCCS(=O)(=O)O</chem>                    |
| InChI                        | SUMDYPCJJOFFON-UHFFFAOYSA-N                   |
| InChIKey                     | 1S/C2H6O4S/c3-1-2-7(4,5)6/h3H,1-2H2,(H,4,5,6) |
| Water solubility             | 1.00E+06 mg/L                                 |
| log P (octanol-water)        | -3.360  |
| Atmospheric OH Rate Constant | 5.45E-12 cm <sup>3</sup> /molecule-sec        |
| Melting Point                | < 25 &deg; C                                  |



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