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## Typical Product Specifications & Properties

# atropic acid

CAS Number: : 492-38-6

| Specifications               | Limits                                                   |
|------------------------------|----------------------------------------------------------|
| Molecular weight             | 148.16                                                   |
| EINECS                       | 207-753-6                                                |
| SMILES                       | <chem>c1ccccc1C(=C)C(=O)O</chem>                         |
| InChI                        | 1S/C9H8O2/c1-7(9(10)11)8-5-3-2-4-6-8/h2-6H,1H2,(H,10,11) |
| InChIKey                     | ONPJWQSDZCGSQM-UHFFFAOYSA-N                              |
| log P (octanol-water)        | 2.210                                                    |
| Atmospheric OH Rate Constant | 2.03E-11 cm <sup>3</sup> /molecule-sec                   |
| Melting Point                | 106.5 &deg; C                                            |
| Water solubility             | 1300 mg/L                                                |



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