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## Typical Product Specifications & Properties

# A,a,a-trifluoro-4-cresol

CAS Number: : 402-45-9

| Specifications               | Limits                                         |
|------------------------------|------------------------------------------------|
| Molecular weight             | 162.11                                         |
| EINECS                       | 206-945-7                                      |
| SMILES                       | <chem>Oc1ccc(C(F)(F)F)cc1</chem>               |
| InChI                        | 1S/C7H5F3O/c8-7(9,10)5-1-3-6(11)4-2-5/h1-4,11H |
| InChIKey                     | BAYGVMXZJBFEMB-UHFFFAOYSA-N                    |
| log P (octanol-water)        | 2.82                                           |
| Henry's Law Constant         | 4.87E-06 atm-m <sup>3</sup> /mole              |
| Melting Point                | 46 &deg; C                                     |
| pKa Dissociation Constant    | 8.675                                          |
| Vapor Pressure               | 0.668 mm Hg                                    |
| Atmospheric OH Rate Constant | 6.84E-12 cm <sup>3</sup> /molecule-sec         |
| Water solubility             | 994 mg/L                                       |



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| Specifications      | Limits              |
|---------------------|---------------------|
| Melting Point       | 45-47 °C            |
| Flash Point         | 183 °F              |
| Storage Temperature | 0-6°C               |
| Boiling Point       | 71.5-72 °C (8 mmHg) |



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