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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-m3/mole
Melting Point	46 ° C
pKa Dissociation Constant	8.675
Vapor Pressure	0.668 mm Hg
Atmospheric OH Rate Constant	6.84E-12 cm3/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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