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Typical Product Specifications & Properties

3-Acetylbenzonitrile

CAS Number: : 6136-68-1

Specifications	Limits
Molecular weight	145.16
EINECS	228-110-6
SMILES	<chem>CC(=O)c1cc(C#N)ccc1</chem>
InChI	1S/C9H7NO/c1-7(11)9-4-2-3-8(5-9)6-10/h2-5H,1H3
InChIKey	SBCFGFDAZCTSRH-UHFFFAOYSA-N
log P (octanol-water)	1.16
Henry's Law Constant	9.48E-08 atm-m3/mole
Vapor Pressure	6.42E-03 mm Hg
Atmospheric OH Rate Constant	4.16E-13 cm3/molecule-sec
Melting Point	98-100 ° C
Water solubility	4420 mg/L
Boiling Point	120 °C (5 mmHg)



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Specifications	Limits
BRN Number	2079629
Flash Point	120°C/5mm
Melting Point	98-100 °C
Water solubility	Insoluble in water.



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