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Typical Product Specifications & Properties

2-Methylbenzonitrile

CAS Number: : 529-19-1

Specifications	Limits
Molecular weight	117.15
EINECS	208-451-7
SMILES	<chem>c1(c(ccc1)C)C#N</chem>
InChI	1S/C8H7N/c1-7-4-2-3-5-8(7)6-9/h2-5H,1H3
InChIKey	NWPNXBQSRGKSJB-UHFFFAOYSA-N
Atmospheric OH Rate Constant	1.03E-12 cm ³ /molecule-sec
log P (octanol-water)	2.21
Boiling Point	205 ° C
Henry's Law Constant	5.74E-05 atm-m ³ /mole
Water solubility	724 mg/L
Melting Point	-1.35E+01 ° C
Flash Point	184 ° F



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Specifications	Limits
Water solubility	<0.1 g/100 mL at 17 °C
Density	0.989 g/mL at 25 °C
Refractive Index	1.5279
Merck	14,9537
Melting Point	-13 °C
Boiling Point	205 °C



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