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Typical Product Specifications & Properties

4-tert-Butylpyridine

CAS Number: : 3978-81-2

Specifications	Limits
Molecular weight	135.21
EINECS	223-614-2
SMILES	<chem>c1(ccncc1)C(C)(C)C</chem>
InChI	1S/C9H13N/c1-9(2,3)8-4-6-10-7-5-8/h4-7H,1-3H3
InChIKey	YSHMQTRICHYLGU-UHFFFAOYSA-N
Henry's Law Constant	1.82E-05 atm-m3/mole
Atmospheric OH Rate Constant	1.32E-12 cm3/molecule-sec
Vapor Pressure	0.972 mm Hg
pKa Dissociation Constant	5.99
Melting Point	-4.10E+01 ° C
log P (octanol-water)	2.710
Boiling Point	196.5 ° C



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Specifications	Limits
Water solubility	422 mg/L
Flash Point	146 °F
Density	0.923 g/mL at 25 °C
Boiling Point	196-197 °C
Refractive Index	1.495



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