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Typical Product Specifications & Properties

4-tert-BUTYLTOLUENE

CAS Number: : 98-51-1

Specifications	Limits
Molecular weight	148.24
EINECS	202-675-9
SMILES	<chem>C(c1ccc(C)cc1)(C)(C)C</chem>
InChI	1S/C11H16/c1-9-5-7-10(8-6-9)11(2,3)4/h5-8H,1-4H3
InChIKey	QCWXDVFBZVHKLV-UHFFFAOYSA-N
Henry's Law Constant	0.015 atm-m ³ /mole
log P (octanol-water)	5.17
Atmospheric OH Rate Constant	1.40E-11 cm ³ /molecule-sec
Melting Point	-5.20E+01 ° C
Vapor Pressure	0.671 mm Hg
Boiling Point	190 ° C
Water solubility	5.500 mg/L



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Specifications	Limits
Water solubility	0.06 g/100 mL (20 °C)
Melting Point	-54 °C
Refractive Index	1.492
Storage Temperature	Flammables area
Solubility	0.06 g/100 mL (20°C)
Density	0.858 g/mL at 25 °C
Boiling Point	191 °C
BRN Number	2038670
Stability	Stable. Combustible. Incompatible with strong oxidizing agents.
Flash Point	150 °F



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