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Typical Product Specifications & Properties

2-(tert-Butyl)phenol

CAS Number: : 88-18-6

Specifications	Limits
Molecular weight	150.22
EINECS	201-807-2
SMILES	<chem>c1(c(ccc1)O)C(C)(C)C</chem>
InChI	1S/C10H14O/c1-10(2,3)8-6-4-5-7-9(8)11/h4-7,11H,1-3H3
InChIKey	WJQOZHYUIDYNHM-UHFFFAOYSA-N
pKa Dissociation Constant	10.28
Water solubility	700 mg/L
Boiling Point	223 ° C
Henry's Law Constant	2.54E-05 atm-m ³ /mole
Atmospheric OH Rate Constant	4.06E-11 cm ³ /molecule-sec
log P (octanol-water)	3.31
Melting Point	-6.80E+00 ° C



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Specifications	Limits
Melting Point	-7 °C
BRN Number	1907120
Water solubility	0.23 g/100 mL (20 °C)
Refractive Index	1.523
Flash Point	>230 °F
Vapor Pressure	0.05 mm Hg (20 °C)
Boiling Point	224 °C
Density	0.978 g/mL at 25 °C



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