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Typical Product Specifications & Properties

4-tert-Butyl-2-nitrophenol

CAS Number: : 3279-07-0

Specifications	Limits
Molecular weight	195.22
EINECS	221-914-8
SMILES	<chem>C(c1cc([N+](=O)[O-])c(O)cc1)(C)(C)C</chem>
InChI	1S/C10H13NO3/c1-10(2,3)7-4-5-9(12)8(6-7)11(13)14/h4-6,12H,1-3H3
InChIKey	IHGNADPMUSNTJW-UHFFFAOYSA-N
Vapor Pressure	6.57E-05 mm Hg
Henry's Law Constant	1.81E-05 atm-m3/mole
log P (octanol-water)	3.820
Water solubility	25.4 mg/L
Atmospheric OH Rate Constant	5.64E-12 cm3/molecule-sec
Flash Point	>230 °F
Melting Point	27-29 °C



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Specifications	Limits
Density	1.12 g/mL at 25 °C
Boiling Point	97 °C/1 mm Hg



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