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Typical Product Specifications & Properties

4-Nitroanisole

CAS Number: : 100-17-4

Specifications	Limits
Molecular weight	153.14
SMILES	<chem>c1(ccc(OC)cc1)[N+](=O)[O-]</chem>
InChI	1S/C7H7NO3/c1-11-7-4-2-6(3-5-7)8(9)10/h2-5H,1H3
InChIKey	BNUHAJGCKIQFGE-UHFFFAOYSA-N
Water solubility	590 mg/L
Atmospheric OH Rate Constant	2.46E-12 cm ³ /molecule-sec
log P (octanol-water)	2.03
pKa Dissociation Constant	-1.00E+01
Boiling Point	274 ° C
Melting Point	54 ° C
Henry's Law Constant	1.26E-06 atm-m ³ /mole
Vapor Pressure	0.019 mm Hg

