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## Typical Product Specifications & Properties

# 4-Nitrophenylacetic Acid

CAS Number: : 104-03-0

Specifications	Limits
Molecular weight	181.15
SMILES	<chem>O=C(O)Cc1ccc([N+](=O)[O-])cc1</chem>
InChI	YBADLXQNJCMCKR-UHFFFAOYSA-N
InChIKey	1S/C8H7NO4/c10-8(11)5-6-1-3-7(4-2-6)9(12)13/h1-4H,5H2,(H,10,11)
Water solubility	3570 mg/L
Henry's Law Constant	1.74E-10 atm-m <sup>3</sup> /mole
Atmospheric OH Rate Constant	1.62E-12 cm <sup>3</sup> /molecule-sec
Melting Point	154 &deg; C
log P (octanol-water)	1.39
Vapor Pressure	2.91E-05 mm Hg
pKa Dissociation Constant	3.85



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415 Huguenot Street, New Rochelle, New York 10801

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