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Typical Product Specifications & Properties

4-Tert-Butylphenylacetic Acid

CAS Number : 32857-63-9

Specifications	Limits
Molecular weight	192.25
EINECS	251-264-0
SMILES	<chem>O=C(O)Cc1ccc(cc1)C(C)(C)C</chem>
InChI	RUAYXHSDAMWEDR-UHFFFAOYSA-N
InChIKey	1S/C12H16O2/c1-12(2,3)10-6-4-9(5-7-10)8-11(13)14/h4-7H,8H2,1-3H3,(H,13,14)
Atmospheric OH Rate Constant	6.15E-12 cm ³ /molecule-sec
Vapor Pressure	2.39E-04 mm Hg
log P (octanol-water)	2.98
Henry's Law Constant	1.14E-07 atm-m ³ /mole
Water solubility	339 mg/L
pKa Dissociation Constant	4.42
Melting Point	77-78°C



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