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Typical Product Specifications & Properties

4-Phenylbutyric Acid

CAS Number: : 1821-12-1

Specifications	Limits
Molecular weight	164.20
EINECS	217-341-8
SMILES	<chem>OC(=O)CCCC1CCCCC1</chem>
InChI	1S/C10H12O2/c11-10(12)8-4-7-9-5-2-1-3-6-9/h1-3,5-6H,4,7-8H2,(H,11,12)
InChIKey	OBKXEAXTFZPCHS-UHFFFAOYSA-N
Boiling Point	165 °C/10 mm Hg
BRN Number	638180
Water solubility	5.3 g/L at 40 °C
Flash Point	>230 °F
Melting Point	49-51 °C



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