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Typical Product Specifications & Properties

3-Phenylbutyric acid

CAS Number: : 4593-90-2

Specifications	Limits
Molecular weight	164.20
EINECS	224-987-4
SMILES	<chem>c1([C@@H](CC(O)=O)C)ccccc1</chem>
InChI	1S/C10H12O2/c1-8(7-10(11)12)9-5-3-2-4-6-9/h2-6,8H,7H2,1H3,(H,11,12)
InChIKey	ZZEWMYILWXCRHZ-UHFFFAOYSA-N
Atmospheric OH Rate Constant	8.25E-12 cm ³ /molecule-sec
Water solubility	2240 mg/L
Henry's Law Constant	7.79E-08 atm-m ³ /mole
log P (octanol-water)	2.18
Melting Point	39-37 °C
Vapor Pressure	1.31E-03 mm Hg
BRN Number	2044322



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Specifications	Limits
Melting Point	35-38 °C
Flash Point	77 °F
Boiling Point	170-172 °C/20 mm Hg
Density	1.515 g/mL at 25 °C



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