

## Typical Product Specifications & Properties

# HIPPURIC ACID

**CAS Number: 495-69-2**

Specifications	Limits
Molecular weight	179.17
SMILES	<chem>c1(C(NCC(O)=O)=O)ccccc1</chem>
InChI	1S/C9H9NO3/c11-8(12)6-10-9(13)7-4-2-1-3-5-7/h1-5H,6H2,(H,10,13)(H,11,12)
InChIKey	QIAFMBKCNZACKA-UHFFFAOYSA-N
log P (octanol-water)	0.31
Water solubility	3750 mg/L
Melting Point	191.5 ° C
Atmospheric OH Rate Constant	1.07E-11 cm <sup>3</sup> /molecule-sec
Vapor Pressure	7.62E-07 mm Hg
Henry's Law Constant	7.21E-13 atm-m <sup>3</sup> /mole