



www.parchem.com

GET A QUICK QUOTE

## Typical Product Specifications & Properties

# Betanine

CAS Number: : 7659-95-2

Specifications	Limits
Molecular weight	550.47
EINECS	231-628-5
SMILES	<chem>OC[C@H]1O[C@@H](Oc2cc3C[C@H](N\C=C\C4=CC(=N[C@@H](C4)C(=O)O)C(=O)O)c3cc2O)C(=O)O)[C@H](O)[C@@H](O)[C@@H]1O</chem>
InChI	CTMLKIKAUFEML-FTNGGYTGSA-N
InChIKey	1S/C24H26N2O13/c27-8-17-18(29)19(30)20(31)24(39-17)38-16-6-10-5-14(23(36)37)26(13(10)7-15(16)28)2-1-9-3-11(21(32)33)25-12(4-9)22(34)35/h1-3,6-7,12,14,17-20,24,27-31H,4-5,8H2,(H,32,33)(H,34,35)(H,36,37)/b2-1+/t12-,14-,17+,18+,19-,20+,24+/m0/s1



GET A QUICK QUOTE

415 Huguenot Street, New Rochelle, New York 10801