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## Typical Product Specifications & Properties

# Neochlorogenic Acid

CAS Number: : 906-33-2

Specifications	Limits
Molecular weight	354.31
EINECS	212-997-1
SMILES	<chem>O(C(\C=C\c1ccc(c(c1)O)O)=O)[C@@H]1C[C@@](C[C@H]([C@@H]1O)O)(C(=O)O)O</chem>
InChI	CWVRJTMFETXNAD-NXLLHMKUSA-N
InChIKey	1S/C16H18O9/c17-9-3-1-8(5-10(9)18)2-4-13(20)25-12-7-16(24,15(22)23)6-11(19)14(12)21/h1-5,11-12,14,17-19,21,24H,6-7H2,(H,22,23)/b4-2+/t11-,12-,14+,16-/m1/s1



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