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## Typical Product Specifications & Properties

# Aucubin

CAS Number: : 479-98-1

Specifications	Limits
Molecular weight	346.33
EINECS	207-540-8
SMILES	<chem>O[C@@H]1C=C([C@H]2[C@@H](OC=C[C@@H]12)O[C@@H]1O[C@H](CO)[C@@H](O)[C@@H](O)[C@H]1O)CO</chem>
InChI	RJWJHRPNHPHBRN-FKVJWERZ SA-N
InChIKey	1S/C15H22O9/c16-4-6-3-8(18)7-1-2-22-14(10(6)7)24-15-13(21)12(20)11(19)9(5-17)23-15/h1-3,7-21H,4-5H2/t7-,8+,9+,10+,11+,12-,13+,14-,15-/m0/s1
log P (octanol-water)	-3.490
Atmospheric OH Rate Constant	2.44E-10 cm <sup>3</sup> /molecule-sec
Water solubility	3.56E+05 mg/L
Alpha	D21 -163.1&deg; (c = 1.6)
Storage Temperature	2-8&deg;C
Melting Point	181&deg;

