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Typical Product Specifications & Properties

Swertiamarine

CAS Number: : 17388-39-5

Specifications	Limits
Molecular weight	374.34
SMILES	<chem>OC[C@H]1O[C@@H](O[C@@H]2OC=C3C(=O)OCC[C@@]3(O)[C@H]2C=C)[C@H](O)[C@@H](O)[C@@H]1O</chem>
InChI	HEYZ WPRKKUGDCR-QBXMEVCASA-N
InChIKey	1S/C16H22O10/c1-2-7-14(24-6-8-13(21)23-4-3-16(7,8)22)26-15-12(20)11(19)10(18)9(5-17)25-15/h2,6-7,9-12,14-15,17-20,22H,1,3-5H2/t7-,9+,10+,11-,12+,14-,15-,16+/m0/s1
Melting Point	113-114°
Storage Temperature	?20°C
Alpha	D20 -127° (c = 1 in 96% ethanol)
Merck	14,9010



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