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## Typical Product Specifications & Properties

# Scleroglucan

CAS Number: : 39464-87-4

Specifications	Limits
EINECS	254-464-6
SMILES	<chem>O[C@H]1[C@@H](O[C@@H]([C@H]([C@@H]1O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O*)O)CO)O)CO[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO)O)CO)*</chem>
Molecular weight	303.35
EINECS	200-090-3
SMILES	<chem>CN1[C@@H]2C[C@H](C[C@H]1[C@H]3[C@@H]2O3)OC(=O)[C@H](CO)c4ccccc4</chem>
InChI	1S/C17H21NO4/c1-18-13-7-11(8-14(18)16-15(13)22-16)21-17(20)12(9-19)10-5-3-2-4-6-10/h2-6,11-16,19H,7-9H2,1H3/t11-,12?,13?,14?,15-,16+
InChIKey	STECJAGHUSJQJN-MBBCWDQXSA-N
Vapor Pressure	7.18E-09 mm Hg
Water solubility	1.00E+05 mg/L
pKa Dissociation Constant	7.75
Atmospheric OH Rate Constant	5.97E-11 cm <sup>3</sup> /molecule-sec
log P (octanol- water)	0.98

ISO 9001



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Specifications	Limits
Henry's Law Constant	3.36E-16 atm-m <sup>3</sup> /mole
Melting Point	59 &deg; C
Molecular weight	398.29
EINECS	205-844-5
SMILES	[Br].C[N+](C)[C@@H]2CC(C[C@H]1[C@@H]3O[C@H]23)OC(=O)[C@H](CO)c4ccccc4
InChI	CXYRUNPLKGGUJF-RAFJPFSSSA-M
InChIKey	1S/C18H24NO4.BrH/c1-19(2)14-8-12(9-15(19)17-16(14)23-17)22-18(21)13(10-20)11-6-4-3-5-7-11;/h3-7,12-17,20H,8-10H2,1-2H3;1H/q+1;/p-1/t12-,13-,14-,15+,16-,17+;/m1./s1
log P (octanol-water)	-2.580



Specifications Limits

Atmospheric  
OH Rate  
Constant

5.50E-11 cm<sup>3</sup>/molecule-sec

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