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Typical Product Specifications & Properties

Sarsasapogenin

CAS Number: : 126-19-2

Specifications	Limits
Molecular weight	416.64
EINECS	204-776-3
InChI	1S/C27H44O3/c1-16-7-12-27(29-15-16)17(2)24-23(30-27)14-22-20-6-5-18-13-19(28)8-10-25(18,3)21(20)9-11-26(22,24)4/h16-24,28H,5-15H2,1-4H3/t16?,17?,18-,19+,20?,21?,22?,23?,24?,25?,26?,27?/m0/s1
InChIKey	GMBQZIIUCVW OCD-NCYQLCQRSA-N
Melting Point	194°C
Merck	13,8456
Molecular weight	280.30
EINECS	211-480-8
SMILES	c1(S(Nc2ncc(OC)cn2)(=O)=O)ccc(N)cc1
InChI	1S/C11H12N4O3S/c1-18-9-6-13-11(14-7-9)15-19(16,17)10-4-2-8(12)3-5-10/h2-7H,12H2,1H3,(H,13,14,15)
InChIKey	GPTONYMQFTZPKC-UHFFFAOYSA-N
Atmospheric OH Rate Constant	2.80E-11 cm ³ /molecule-sec



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Specifications	Limits
Melting Point	214-216 ° C
Water solubility	730 mg/L
log P (octanol-water)	0.41
Henry's Law Constant	9.36E-12 atm-m ³ /mole
Vapor Pressure	8.35E-09 mm Hg
Color	white with faint yellow cast
Melting Point	214-216°C
Storage Temperature	2-8°C
Merck	13,8999



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