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Typical Product Specifications & Properties

Tigogenin

CAS Number: : 77-60-1

Specifications	Limits
Molecular weight	416.64
EINECS	201-041-9
SMILES	<chem>C[C@@H]1CC[C@@]2(OC1)O[C@H]3C[C@H]4[C@@H]5CC[C@](O)CC[C@]6(C)[C@H]5CC[C@]4(C)[C@H]3[C@@H]2C</chem>
InChI	1S/C27H44O3/c1-16-7-12-27(29-15-16)17(2)24-23(30-27)14-22-219(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-PODJHBEMSA-N
Atmospheric OH Rate Constant	7.00E-11 cm ³ /molecule-sec
Melting Point	205.5 ° C
log P (octanol-water)	7.110
Melting Point	202-204°C
Alpha	-68 ° (c=0.8g/100ml, CHCl ₃)



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