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Typical Product Specifications & Properties

(6E,22E)-(3R)-9,10-secoergosta-5(10),6,8,22-tetraen-3-ol

CAS Number: : 115-61-7

Specifications	Limits
Molecular weight	396.65
EINECS	204-096-7
SMILES	<chem>CC1=C(C[C@H](CC1)O)/C=C/C2=CCC[C@]3([C@H]2CC[C@@H]3[C@H](C)/C=C/[C@H](C)C(C)C)C</chem>
InChI	XQFJZHAVTPYDIQ-LETJEVNCSA-N
InChIKey	1S/C28H44O/c1-19(2)20(3)9-10-22(5)26-15-16-27-23(8-7-17-28(26,27)6)12-13-24-18-25(29)14-11-21(24)4/h8-10,12-13,19-20,22,25-27,29H,7,11,14-18H2,1-6H3/b10-9+,13-12+/t20-,22+,25-,26+,27-,28+/m0/s1
log P (octanol-water)	10.36
Melting Point	< 25 ° C
Atmospheric OH Rate Constant	3.82E-10 cm ³ /molecule-sec



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415 Huguenot Street, New Rochelle, New York 10801

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