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Typical Product Specifications & Properties

(3β,4α,16α)-3,16-dihydroxy-23-oxoolean-12-en-28-oic acid

CAS Number: : 631-01-6

Specifications	Limits
Molecular weight	486.68
EINECS	211-149-8
SMILES	<chem>C=12[C@@H]3CC(C)(C)CC[C@]3(C(=O)O)[C@@H](C[C@@]2([C@@]2([C@@H]([C@@]3CC[C@H]([C@@]([C@@H]3CC2)(C=O)C)O)C)CC1)C)O</chem>
InChI	MQUFAARYGOUYEV-UAWZMHPWSA-N
InChIKey	1S/C30H46O5/c1-25(2)13-14-30(24(34)35)19(15-25)18-7-8-21-26(3)11-10-22(32)27(4,17-31)20(26)9-12-28(21,5)29(18,6)16-23(30)33/h7,17,19-23,32-33H,8-16H2,1-6H3,(H,34,35)/t19-,20+,21+,22-,23+,26-,27-,28+,29+,30+/m0/s1
Melting Point	294 ° C
log P (octanol-water)	5.330
Atmospheric OH Rate Constant	1.83E-10 cm ³ /molecule-sec



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415 Huguenot Street, New Rochelle, New York 10801

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