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Typical Product Specifications & Properties

1,-dihydro-7-isopropyl-3-[3-[5-isopropyl-3,8-dimethylazulen-1-yl]-2-oxido-4-oxocyclobut-2-en-1-ylide

CAS Number: : 12157-31-2

Specifications	Limits
Molecular weight	446.58
EINECS	235-278-4
SMILES	<chem>CC(C)C1=CC=CC2C(=C1)C=[C+]/C/2=C/3\C(=C(C3=O)c4cc(C)c5cc(ccc(C)c45)C(C)C[O-]</chem>
InChI	RCVVHSPIAFFKHS-UHFFFAOYSA-N
InChIKey	1S/C32H30O2/c1-17(2)21-8-7-9-24-23(15-21)12-13-25(24)29-31(33)30(32(29)34)27-14-20(6)26-16-22(18(3)4)11-10-19(5)28(26)27/h7-12,14-18,24H,1-6H3



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