

(1R,3AS,5AR,5BR,7AR,9S,11AR,11BR,13AR,13BR)-9-HYDROXY-5A,5B,8,8,11A-PENTAMETHYL-1-(PROP-1-EN-2-YL)-ICOSAHYDRO-1H-CYCLOPENTA[A]CHRYSENE-3A-CARBOXYLIC ACID

Catalog Id:

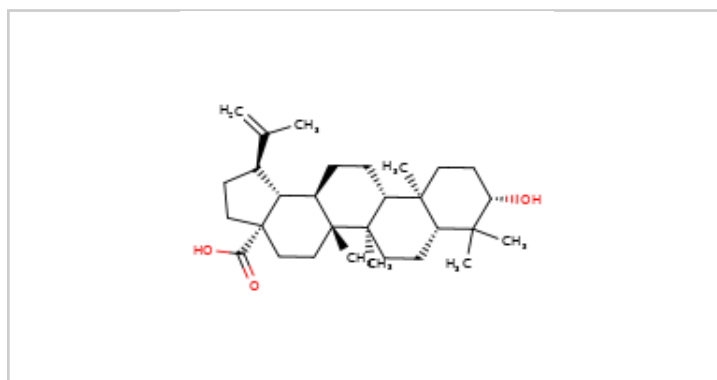
MM472151

IUPAC:

BETULINICACID

CAS Number:

472-15-1



More Information:

Molecular Weight: 456.711

Formula: C₃₀H₄₈O₃

SMILES:

CC(=C)[C@@H]1CC[C@@]2(CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC[C@H](O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12)C(O)=O

Preferred IUPAC Name: (1R,3AS,5AR,5BR,7AR,9S,11AR,11BR,13AR,13BR)-9-HYDROXY-5A,5B,8,8,11A-PENTAMETHYL-1-(PROP-1-EN-2-YL)-ICOSAHYDRO-1H-CYCLOPENTA[A]CHRYSENE-3A-CARBOXYLIC ACID

InChIKey: InChIKey=QGJZLNKBHJESQX-FZFNOLFKSA-N