



Formula: C<sub>20</sub>H<sub>28</sub>O<sub>2</sub>

MW: 300.44

CAS: 302-79-4

TNP NUMBER: TNP00194

MDL NUMBER: MFCD00001551

IUPAC: (2E,4E,6E,8E)-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-enyl)nona-2,4,6,8-tetraenoic acid

Smiles: C1(/C=CC(=C/C=CC(=C/C(=O)O)C)C)=C(CCCC1(C)C)C

ACCEPTORS: 2

DONORS: 1

ROTATION BONDS: 6

N+O: 2

Chiral Centers: 0

LogP: 7.31

LogS: -5.56

LIPINSKI: 3

Synonyms: TRETINOIN;TRETINOIN VITAMIN A ACID;TRANS-RETINOIC ACID;TRANS VITAMIN A ACID;VITAMIN A ACID;VITAMIN A ACID, ALL-TRANS;RETINOIC ACID;RETINOIC ACID, ALL TRANS

CAS:302-79-4

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MW:300.44

EINECS:206-129-0

Product Categories:PHARMACEUTICALS;Active Pharmaceutical Ingredients;APIs;Biochemistry;Terpenes;Terpenes (Others);Vitamins;Intermediates & Fine Chemicals;Retinoids;Intracellular receptor Tretinoin

Chemical Properties: mp 180-181 C(lit.) storage temp. 2-8C form powder color yellow Water Solubility insoluble Merck 14,8165 BRN 2057223

CAS DataBase Reference: 302-79-4(

CAS DataBase Reference: ) EPA Substance Registry SystemRetinoic acid(302-79-4) T,Xn Risk Statements 22-63-38-20/21/22 Safety Statements 53-26-36/37/39-45-36/37 RIDADR 3249 WGK Germany 3 RTECS VH6475000 F 7-8-16-23 HazardClass 6.1(b) PackingGroup III Hazardous Substances Data302-79-4(Hazardous Substances Data) 3,7-Dimethyl-9-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2,4,6,8-nonatetraenoic acid Tretinoin

Usage And Synthesis:

Chemical Properties: Yellow-Orange Powder UsagePhysiological metabolite of vitamin A. Effects gene expression via nuclear retinoic acid receptors (RAR); mediates cellular growth and differentiation General DescriptionYellow to light-orange crystalline powder. Air & Water ReactionsTretinoin may be sensitive to prolonged exposure to air. Insoluble in water. Reactivity ProfileTretinoin may discolor on exposure to light. Tretinoin is extremely sensitive to exposure to light and, therefore, Tretinoin should be fully protected from light during all handling. Solutions are unstable in the presence of strong oxidizers. Tretinoin is incompatible with strong oxidizing agents. . Fire HazardFlash point data for Tretinoin are not available; however, Tretinoin is probably combustible. Biological ActivityEndogenous agonist for retinoic acid receptors. Also

positively modulates PPAR  $\delta$  receptors ( $K_d = 17$  nM). Promotes differentiation of embryonic stem cells (ESCs) into adipocytes, neurons and glia in vitro . Tretinoin

