



Formula: C<sub>27</sub>H<sub>33</sub>N<sub>3</sub>O<sub>8</sub>

MW: 527.57

CAS: 751-97-3

TNP NUMBER: TNP00615

MDL NUMBER: MFCD03548029

IUPAC: [(4S,6S,12aS,4aS,5aS)-4-(dimethylamino)-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo(4,5,6,12a,4a,5a-hexahydronaphthacen-2-yl)]-N-(pyrrolidinylmethyl)carb oxamide

Smiles:

C12=C([C]3(C(C(=C(O)[C@H]([C@@H]3(C[C@@H]2([C@@](O)(C)c2c(C1=O)c(O)ccc2)))N(C)C)C(NCN1CCCC1)=O)=O)O

Semisynthetic antibiotic prepared from tetracycline; Used as antibacterial, administered intravenously or intramuscularly

THERAPEUTIC CATEGORY: Antibacterial

ACCEPTORS: 8

DONORS: 6

ROTATION BONDS: 5

N+O: 11

Chiral Centers: 5

LogP: 0.12

LogS: -4.01

LIPINSKI: 2

Synonyms:

12,12a-pentahydroxy-6-methyl-1,11-dioxo-n-(1-pyrrolidinylmethyl)-1;bristacin;n-(1-pyrrolidinylmethyl)-tetracycline;n-(pyrrolidinomethyl)tetracycline;pirrolidinometil-tetraciclina;prm-tc;pyrrolidino methyl-tetracyclin;pyrrolidino-methyl-tetracycline

CAS:751-97-3

MF:C27H33N3O8

MW:527.57

EINECS:212-031-9

Product Categories: ROLITETRACYCLINE Hazard Codes Xn Risk Statements 22-36/37/38  
Safety Statements 26-36 WGK Germany 1 RTECS Q19150000 ROLITETRACYCLINE

Usage And Synthesis: ROLITETRACYCLINE

