



Formula: C<sub>30</sub>H<sub>40</sub>N<sub>4</sub>

MW: 456.67

Salt: 2Cl<sup>-</sup>, H<sub>2</sub>O

CAS: 522-51-0

MDL NUMBER: MFCD04112822

IUPAC: 1-[10-(4-amino-2-methylquinolyl)decyl]-2-methyl-4-quinolylamine

Smiles: C(CCCCCCCC[n+]1c2c(c(cc1C)N)cccc2)[n+]1c2c(c(cc1C)N)cccc2

THERAPEUTIC CATEGORY: Antiseptic, Disinfectant

REFERENCE: Merck 13, 2930 Dunn PM. Dequalinium, a selective blocker of the slow afterhyperpolarization in rat sympathetic neurones in culture. Eur J Pharmacol. 1994 Feb 3;252(2):189-94 Bleday R, et al. Inhibition of rat colon tumor isograft growth with dequalinium chloride. Arch Surg. 1986 Nov;121(11):1272-5

ACCEPTORS: 0

DONORS: 4

ROTATION BONDS: 11

N+O: 4

Chiral Centers: 0

LogP: 4.98

LogS: -4.03

LIPINSKI: 4

Synonyms: METHYL VIOLOGEN DICHLORIDE HYDRATE;METHYL VIOLOGEN HYDRATE;1,1'-DIMETHYL-4,4'-BIPYRIDINIUM DICHLORIDE HYDRATE;PARAQUAT HYDRATE;PARAQUAT DICHLORIDE HYDRATE

CAS:

MF:C12H16Cl2N2O

MW:275.17

EINECS:217-615-7

Product Categories: 1,1'-DIMETHYL-4,4'-BIPYRIDINIUM DICHLORIDE HYDRATE

Chemical Properties: mp >300 C(lit.) storage temp. APPROX 4C T+,N Risk Statements 24/25-26-36/37/38-48/25-50/53 Safety Statements 22-28-36/37/39-45-60-61 RIDADR UN 2811 6.1/PG 1 WGK Germany 3 RTECS DW2275000 1,1'-DIMETHYL-4,4'-BIPYRIDINIUM DICHLORIDE HYDRATE

Usage And Synthesis: 1,1'-DIMETHYL-4,4'-BIPYRIDINIUM DICHLORIDE HYDRATE

