



Formula: C₂₃H₂₃IN₂S₂

MW: 518.49

CAS: 514-73-8

MDL NUMBER: MFCD00074829

IUPAC: 2-[(1E,3E)-5-(3-ethyl(3-hydrobenzothiazol-2-ylidene))penta-1,3-dienyl]-3-ethylbenzothiazole, iodide

Smiles: [n+]1(c(sc2c1cccc2)/C=CC=C/C=C1/n(c2ccccc2s1)CC)CC.[I-]

Powder

THERAPEUTIC CATEGORY: Anthelmintic (Nematodes)

ACCEPTORS: 0

DONORS: 0

ROTATION BONDS: 5

N+O: 2

Chiral Centers: 0

LogP: 9.29

LogS: -6.5

LIPINSKI: 2

Synonyms: DELVEX;DEJO;COMPOUND 01748;EASTMAN 7663;DILOMBRIN;DILOMBRINE;DIETHYLTHIADICARBOCYANINE IODIDE;DITHIAZANINE IODIDE

CAS:514-73-8

MF:C23H23IN2S2

MW:518.48

EINECS:208-186-7

Product Categories: 3,3'-DIETHYLTHIADICARBOCYANINE IODIDE

Chemical Properties: mp 249 C (dec.)(lit.) storage temp. Poison room Merck 14,3369 BRN 3838938 T+ Risk Statements 28-36/37/38 Safety Statements 26-28-36/37-45 RIDADR UN 2811 6.1/PG 2 WGK Germany 3 RTECS DL7060000 F 8 HazardClass 6.1 PackingGroup II 3,3'-DIETHYLTHIADICARBOCYANINE IODIDE

Usage And Synthesis:

Chemical Properties: green crystalline powder General DescriptionGreen, needle-like crystals. Used as a veterinary anthelmintic, as a sensitizer for photographic emulsions and as an insecticides. Not registered as a pesticide in the U.S. Reactivity ProfileAn amine, organosulfide. Organosulfides are incompatible with acids, diazo and azo compounds, halocarbons, isocyanates, aldehydes, alkali metals, nitrides, hydrides, and other strong reducing agents. Reactions with these materials generate heat and in many cases hydrogen gas. Many of these compounds may liberate hydrogen sulfide upon decomposition or reaction with an acid. Amines are chemical bases. They neutralize acids to form salts plus water. These acid-base reactions are exothermic. The amount of heat that is evolved per mole of amine in a neutralization is largely independent of the strength of the amine as a base. Amines may be incompatible with isocyanates, halogenated organics, peroxides, phenols (acidic), epoxides, anhydrides, and acid halides. Flammable gaseous hydrogen is generated by amines in combination with strong reducing agents, such as hydrides. Health HazardHighly toxic by mouth. (Non-Specific -- Pesticide, Solid, n.o.s.) Poisonous if swallowed, or if dust is inhaled. Fire HazardWhen heated to decomposition, 3,3'-DIETHYLTHIADICARBOCYANINE IODIDE emits toxic fumes of iodine, sulfur oxides, and nitrogen oxides. 3,3'-DIETHYLTHIADICARBOCYANINE IODIDE

