

SODIUM 6-CHLORO-2-[(1E)-3-[(2Z)-5-CHLORO-3-ETHYL-1-(3-SULFONATOPROPYL)-6-(TRIFLUOROMETHYL)-2,3-DIHYDRO-1H-1,3-BENZODIAZOL-2-YLIDENE]PROP-1-EN-1-YL]-1-ETHYL-3-(3-SULFONATOPROPYL)-5-(TRIFLUOROMETHYL)-1H-1,3-BENZODIAZOL-3-IUM

Catalog Id:

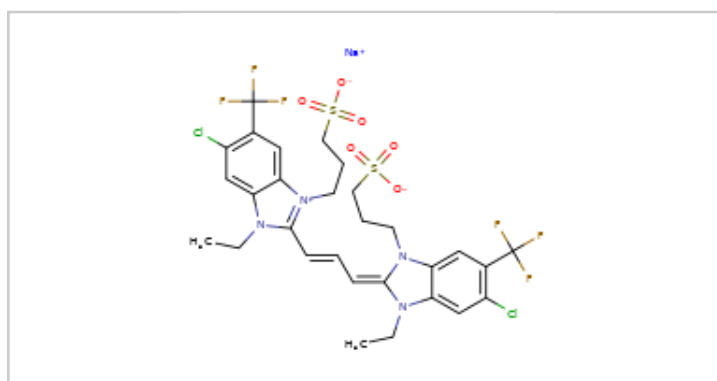
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IUPAC:

SODIUM 3-[5-CHLORO-2-[(E,Z)-3-[6-CHLORO-1-ETHYL-3-(3-SULFONATOPROPYL)-5-(TRIFLUOROMETHYL)BENZIMIDAZOL-2-YLIDENE]PROP-1-ENYL]-3-ETHYL-6-(TRIFLUOROMETHYL)BENZIMIDAZOL-1-IUM-1-YL]PROPANE-1-SULFONATE

CAS Number:

33628-05-6



More Information:

Molecular Weight: 801.57

Formula: C₂₉H₂₉Cl₂F₆N₄NaO₆S₂

SMILES: [Na+].CCN1\C(=C\C=C\C2=[N+](CCCS([O-])(=O)=O)C3=CC(=C(Cl)C=C3N2CC)C(F)(F)F)N(CCCS([O-])(=O)=O)C2=CC(=C(Cl)C=C12)C(F)(F)F

Preferred IUPAC Name: SODIUM 6-CHLORO-2-[(1E)-3-[(2Z)-5-CHLORO-3-ETHYL-1-(3-SULFONATOPROPYL)-6-(TRIFLUOROMETHYL)-2,3-DIHYDRO-1H-1,3-BENZODIAZOL-2-YLIDENE]PROP-1-EN-1-YL]-1-ETHYL-3-(3-SULFONATOPROPYL)-5-(TRIFLUOROMETHYL)-1H-1,3-BENZODIAZOL-3-IUM

InChIKey: InChIKey=XJTFGUSFOPRUQV-UHFFFAOYSA-M