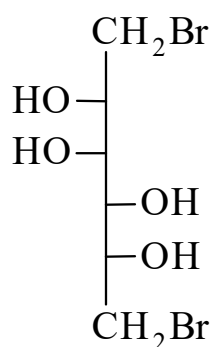




>>Entry Name: 1,6-Dibromo-1,6-dideoxymannitol, 9CI, 8CI

Synonym(s): Mitobronitol, BAN, INN, JAN. Myebrol. Myelobromol. DBM. NSC 94100. WR 220057



Molecular Formula: C₆H₁₂Br₂O₄

Molecular Weight: 307.966

Accurate Mass: 305.950232

Percentage Composition: C 23.40%; H 3.93%; Br 51.89%; O 20.78%

Use/Importance: Alkylating agent; antineoplastic agent

Calculated Log P Data: Log P -2 (calc)

>>Variant: D-form

CAS Registry Number: 488-41-5

Molecular Formula: C₆H₁₂Br₂O₄

Molecular Weight: 307.966

Accurate Mass: 305.950232

Percentage Composition: C 23.40%; H 3.93%; Br 51.89%; O 20.78%

Physical Description: Cryst. (MeOH/dichloroethane)

Melting Point: Mp 176-178°

Hazard & Toxicity: Human systemic effects when used therapeutically. Exp. reprod. and teratogenic effects. LD₅₀ (rat, orl) 1500 mg/kg

Sigma: D4393

>>Derivative: 3,4-*O*-Isopropylidene

Synonym(s): 1,6-Dibromo-1,6-dideoxy-3,4-*O*-isopropylidene-D-mannitol

Molecular Formula: C₉H₁₆Br₂O₄

Molecular Weight: 348.031

Accurate Mass: 345.981532

Percentage Composition: C 31.06%; H 4.63%; Br 45.92%; O 18.39%

Melting Point: Mp 71-72°

Optical Rotation: [α]_D²⁰ +32.8 (Me₂CO)

>>Derivative: 3,4-*O*-Isopropylidene, 2,5-di-Ac

Molecular Formula: C₁₃H₂₀Br₂O₆

Molecular Weight: 432.105

Accurate Mass: 430.002662

Percentage Composition: C 36.14%; H 4.67%; Br 36.98%; O 22.22%

Melting Point: Mp 49-50°

Optical Rotation: [α]_D²⁰ +13.4 (CHCl₃)

>>Derivative: 3,4-*O*-Isopropylidene, 2,5-dimesyl

Melting Point: Mp 112-113°

Optical Rotation: [α]_D²⁰ -1.9 (dioxan)

>>Derivative: Tetramesyl

Melting Point: Mp 105-107°

Optical Rotation: [α]_D²⁰ +29.1 (c, 1.0 in CHCl₃)

References: