



CAS Registry Number: 23031-32-5

Melting Point: Mp 246-248°

Hazard & Toxicity: LD₅₀ (rat, orl) 8700 mg/kg. Exp. reprod. effects

Sigma: T2528

>> **Derivative:** 3,5-Bis(dimethylcarbamate)

Synonym(s): Terbutaline bis(dimethylcarbamate). **Bambuterol**, BAN, INN. KWD 2183. Bambec

CAS Registry Number: 81732-65-2

Molecular Formula: C₁₈H₂₉N₃O₅

Molecular Weight: 367.444

Accurate Mass: 367.210722

Percentage Composition: C 58.84%; H 7.95%; N 11.44%; O 21.77%

Biological Use/Importance: β₂-Adrenoceptor agonist, antiasthmatic, bronchodilator

Development Status: Launched 1990

Calculated Log P Data: Log P 0.56 (calc)

>> **Derivative:** 3,5-Bis(4-methylbenzoyl)

Synonym(s): Terbutaline di(*p*-toluate). **Tobuterol**, INN

CAS Registry Number: 75626-99-2

Molecular Formula: C₂₈H₃₁NO₅

Molecular Weight: 461.557

Accurate Mass: 461.220224

Percentage Composition: C 72.86%; H 6.77%; N 3.03%; O 17.33%

Biological Use/Importance: Bronchodilator

Calculated Log P Data: Log P 5.94 (calc)

>> **Derivative:** 3,5-Bis(2-methylpropanoyl)

Synonym(s): Terbutaline diisobutyrate. **Ibuterol**, INN. Spiranyl

CAS Registry Number: 53034-85-8

Biological Use/Importance: Bronchodilator, smooth muscle relaxant

Development Status: Never marketed

Calculated Log P Data: Log P 2.36 (calc)

>> **Derivative:** 3,5-Bis(2-methylpropanoyl); hydrobromide

Synonym(s): KWD 2058

CAS Registry Number: 52223-83-3

Melting Point: Mp 168-170°

>> **Derivative:** 3,5-Bis(2,2-dimethylpropanoyl)

Synonym(s): Terbutaline dipivalate. **Divabuterol**, INN

CAS Registry Number: 54592-27-7

Molecular Formula: C₂₂H₃₅NO₅

Molecular Weight: 393.522

Accurate Mass: 393.251524

Percentage Composition: C 67.15%; H 8.96%; N 3.56%; O 20.33%

Biological Use/Importance: Bronchospasmolytic, uterine relaxant

Calculated Log P Data: Log P 3.16 (calc)

>> **Derivative:** 3,5-Bis(2,2-dimethylpropanoyl); hydrobromide

Synonym(s): KWD 2085

CAS Registry Number: 52223-87-7

Physical Description: Cryst. (CHCl₃/Et₂O/petrol)

Melting Point: Mp 190-192°

References: