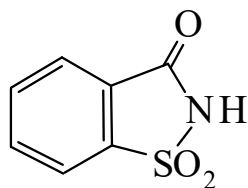




>>Entry Name: Saccharin, USAN

ENTRY UNDER REVIEW

Synonym(s): 1,2-Benzisothiazol-3(2*H*)-one 1,1-dioxide, 9CI. Benzoic sulfimide. *o*-Benzosulfimide. Benzosulfonide. *o*-Benzoylsulfimide. *o*-Sulfobenzoic imide. Garantose. Hermesetas. Sweeta. E 954. FEMA 2998



CAS Registry Number: 81-07-2

Related CAS Registry Numbers(s): 6155-57-3 6381-91-5

Molecular Formula: C₇H₅NO₃S

Molecular Weight: 183.187

Accurate Mass: 182.999014

Percentage Composition: C 45.90%; H 2.75%; N 7.65%; O 26.20%; S 17.50%

Use/Importance: All salts intensely sweet. Widely-used sweetening agent. Used as 25% aq. soln. of Na salt for detn. of Tl; extraction-separation of Ag. Permitted in foods at levels of 80-1200 ppm in EU

Physical Description: Cryst. (H₂O)

Melting Point: Mp 224°

Solubility: Spar. sol. H₂O, EtOH, Me₂CO; sl. sol. Et₂O, CHCl₃

pKa Value: pK_{a1} 1.31 (25°, 0.2M KCl/HCl)

Calculated Log P Data: Log P 0.52 (uncertain value) (calc)

Other Data: Sweetness approx. 300 x sucrose

Hazard & Toxicity: Possible human carcinogen (IARC classification, 1987). LD₅₀ (mus, orl) 17000 mg/kg. Exp. carcinogenic data. Exp. reprod. and teratogenic effects

Aldrich: 10918-5

Fluka: 12475

Rare Chemicals Library: S27211-6

>>Derivative: Na salt

Synonym(s): Saccharin sodium, USAN. Sucaryl

CAS Registry Number: 128-44-9

Melting Point: Mp 228.8-229.7°

Hazard & Toxicity: Possible human carcinogen (IARC classification, 1987). LD₅₀ (rat, orl) 14200 mg/kg. Exp. carcinogen. Exp. reprod. and teratogenic effects

>>Derivative: Ca salt (2:1)

Synonym(s): Saccharin calcium, USAN

CAS Registry Number: 6485-34-3

>>Derivative: Oxime

CAS Registry Number: 51674-07-8

Molecular Formula: C₇H₆N₂O₃S

Molecular Weight: 198.202

Accurate Mass: 198.009913

Percentage Composition: C 42.42%; H 3.05%; N 14.13%; O 24.22%; S 16.18%

Melting Point: Mp 208-210 dec.°

>>Derivative: Benzoyl

CAS Registry Number: 37952-93-5

Molecular Formula: C₁₄H₉NO₄S

Molecular Weight: 287.295

Accurate Mass: 287.025229

Percentage Composition: C 58.53%; H 3.16%; N 4.88%; O 22.28%; S 11.16%

Melting Point: Mp 250 dec.°