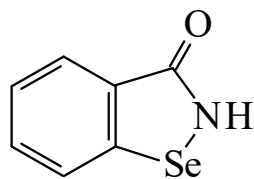




>>Entry Name: 1,2-Benzisoselenazol-3(2*H*)-one, 9CI



CAS Registry Number: 4032-78-4

Molecular Formula: C₇H₅NOSe

Molecular Weight: 198.083

Accurate Mass: 198.953634

Percentage Composition: C 42.45%; H 2.54%; N 7.07%; O 8.08%; Se 39.86%

Physical Description: Needles or plates

Melting Point: Mp 234-235°

>>Derivative: *N*-Me

Molecular Formula: C₈H₇NOSe

Molecular Weight: 212.109

Accurate Mass: 212.969284

Percentage Composition: C 45.30%; H 3.33%; N 6.60%; O 7.54%; Se 37.23%

Melting Point: Mp 156-158 dec.°

>>Derivative: *N*-*tert*-Butyl

Molecular Formula: C₁₁H₁₃NOSe

Molecular Weight: 254.19

Accurate Mass: 255.016234

Percentage Composition: C 51.98%; H 5.15%; N 5.51%; O 6.29%; Se 31.06%

Melting Point: Mp 153°

>>Derivative: *N*-Ph

Synonym(s): 2-Phenyl-1,2-benzisoselenazol-3(2*H*)-one, 9CI. **Ebselen**, INN. PZ 51

CAS Registry Number: 60940-34-3

Molecular Formula: C₁₃H₉NOSe

Molecular Weight: 274.18

Accurate Mass: 274.984934

Percentage Composition: C 56.95%; H 3.31%; N 5.11%; O 5.84%; Se 28.80%

Biological Use/Importance: Catalyst for oxidation of glutathione by hydroperoxides. Antiinflammatory, antioxidant. Used in treatment of liver disorders. Under investigation as a neuroprotectant in stroke

Physical Description: Needles (EtOH)

Melting Point: Mp 182-183° (179-180°)

Sigma: E3520

>>Derivative: *N*-Ph, *Se*-oxide

CAS Registry Number: 104473-83-8

Molecular Formula: C₁₃H₉NO₂Se

Molecular Weight: 290.18

Accurate Mass: 290.979849

Percentage Composition: C 53.81%; H 3.13%; N 4.83%; O 11.03%; Se 27.21%

Use/Importance: Reacts with thiols to give thiocarbonyl cpds.

Melting Point: Mp 180-181°

References: