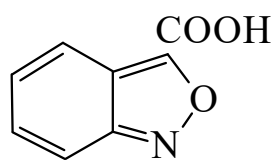




>>Entry Name: **2,1-Benzisoxazole-3-carboxylic acid**, 9CI
Synonym(s): Anthroxanic acid. Anthranil-3-carboxylic acid



CAS Registry Number: 642-91-1

Molecular Formula: C₈H₅NO₃
Molecular Weight: 163.132
Accurate Mass: 163.026944
Percentage Composition: C 58.90%; H 3.09%; N 8.59%; O 29.42%
Melting Point: Mp 198 dec.°
Other Data: Loses CO₂ at 198°, resolidifies and remelts at 245°

>>Derivative: Me ester

Molecular Formula: C₉H₇NO₃
Molecular Weight: 177.159
Accurate Mass: 177.042594
Percentage Composition: C 61.02%; H 3.98%; N 7.91%; O 27.09%
Melting Point: Mp 70°

>>Derivative: Et ester

Molecular Formula: C₁₀H₉NO₃
Molecular Weight: 191.186
Accurate Mass: 191.058244
Percentage Composition: C 62.82%; H 4.74%; N 7.33%; O 25.11%
Melting Point: Mp 64-65°

>>Derivative: Chloride

Molecular Formula: C₈H₄ClNO₂
Molecular Weight: 181.578
Accurate Mass: 180.993056
Percentage Composition: C 52.92%; H 2.22%; Cl 19.52%; N 7.71%; O 17.62%
Melting Point: Mp 44°

>>Derivative: Amide

Molecular Formula: C₈H₆N₂O₂
Molecular Weight: 162.148
Accurate Mass: 162.042928
Percentage Composition: C 59.26%; H 3.73%; N 17.28%; O 19.73%
Physical Description: Cryst. (H₂O)
Melting Point: Mp 211-212°

>>Derivative: Nitrile

Synonym(s): 3-Cyanoanthranil

Molecular Formula: C₈H₄N₂O
Molecular Weight: 144.132
Accurate Mass: 144.032363
Percentage Composition: C 66.67%; H 2.80%; N 19.44%; O 11.10%
Physical Description: Cryst. (Me₂CO)
Melting Point: Mp 58-59°
Boiling Point: Bp₁₁ 50° subl.

References:

Grob, C.A. *et al.*, *Helv. Chim. Acta*, 1961, **44**, 1758, (*synth*)
Eckroth, D.R. *et al.*, *J.C.S.(C)*, 1970, 2660, (*synth*)