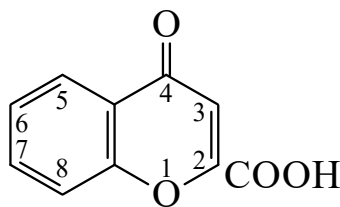




>>Entry Name: 4-Oxo-4*H*-1-benzopyran-2-carboxylic acid, 9Cl, 8Cl
Synonym(s): Chromone-2-carboxylic acid. **Chromocarb**, INN. Atremon



CAS Registry Number: 4940-39-0
Related CAS Registry Numbers(s): 23915-80-2

Molecular Formula: C₁₀H₆O₄
Molecular Weight: 190.155
Accurate Mass: 190.02661
Percentage Composition: C 63.16%; H 3.18%; O 33.66%
Use/Importance: Medicinal intermediate, spasmolytic agent
Physical Description: Cryst. (EtOH)
Melting Point: Mp 260 dec.°
Solubility: Spar. sol. H₂O; insol. Et₂O, CS₂
Calculated Log P Data: Log P 0.63 (calc)

Aldrich: 18978-2
Sigma: O8755

>>Derivative: Me ester

CAS Registry Number: 18398-73-7
Molecular Formula: C₁₁H₈O₄
Molecular Weight: 204.182
Accurate Mass: 204.04226
Percentage Composition: C 64.71%; H 3.95%; O 31.34%
Physical Description: Needles (MeOH)
Melting Point: Mp 122-123°

>>Derivative: Et ester

CAS Registry Number: 14736-31-3
Molecular Formula: C₁₂H₁₀O₄
Molecular Weight: 218.209
Accurate Mass: 218.05791
Percentage Composition: C 66.05%; H 4.62%; O 29.33%
Physical Description: Needles (EtOH)
Melting Point: Mp 69-70° (64-65°)

>>Derivative: Chloride

CAS Registry Number: 5112-47-0
Molecular Formula: C₁₀H₅ClO₃
Molecular Weight: 208.6
Accurate Mass: 207.992722
Percentage Composition: C 57.58%; H 2.42%; Cl 17.00%; O 23.01%
Physical Description: Cryst. (petrol or C₆H₆)
Melting Point: Mp 108-109° (106°)

>>Derivative: Amide

CAS Registry Number: 33543-89-4
Molecular Formula: C₁₀H₇NO₃
Molecular Weight: 189.17
Accurate Mass: 189.042594
Percentage Composition: C 63.49%; H 3.73%; N 7.40%; O 25.37%
Physical Description: Yellow prisms (H₂O or EtOH)
Melting Point: Mp 250-251° (softens 230°)