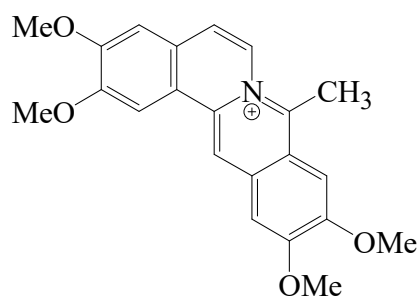




>>Entry Name: Coralyne

Synonym(s): 2,3,10,11-Tetramethoxy-8-methyldibenzo[*a,g*]quinolizinium, 9Cl



CAS Registry Number: 6872-73-7

Molecular Formula: C₂₂H₂₂NO₄⁽⁺⁾

Molecular Weight: 364.42

Accurate Mass: 364.154884

Percentage Composition: C 72.51%; H 6.08%; N 3.84%; O 17.56%

Source/Synthesis: Synthetic compound important in studies of leukaemia

Calculated Log P Data: Log P 0.2 (uncertain value) (calc)

UV: [neutral] λ_{max} 220 (ε 24550); 233 (ε 23440); 243 (ε 20900); 286 (ε 38300); 300 (ε 54950); 310 (ε 60260); 327 (ε 45700); 361 (ε 8710); 405 (ε 14800); 425 (ε 19500) (MeOH) (Berdy) [neutral] λ_{max} 234 (); 241 (); 284 (); 300 (); 310 (); 325 (); 360 (); 405 (); 425 () (EtOH) (Berdy)

>>Derivative: Chloride

CAS Registry Number: 38989-38-7

Molecular Formula: C₂₂H₂₂ClNO₄

Molecular Weight: 399.873

Accurate Mass: 399.123736

Percentage Composition: C 66.08%; H 5.55%; Cl 8.87%; N 3.50%; O 16.00%

Physical Description: Pale yellow cryst. + ½H₂O (EtOH) or amorph. solid

Melting Point: Mp 230° (215° dec.). Mp 183-185° (amorph.)

>>Derivative: Iodide

Molecular Formula: C₂₂H₂₂INO₄

Molecular Weight: 491.325

Accurate Mass: 491.059357

Percentage Composition: C 53.78%; H 4.51%; I 25.83%; N 2.85%; O 13.03%

Physical Description: Golden-yellow cryst.

Melting Point: Mp 263°

References:

Pictet, A. *et al.*, *Ber.*, 1913, **46**, 2688-2697, (*synth*)

Zee-Cheng, K.Y. *et al.*, *J. Pharm. Sci.*, 1972, **61**, 969-971, (*synth*)

Kametani, T. *et al.*, *Chem. Pharm. Bull.*, 1976, **24**, 2525-2531, (*synth, uv, ir*)

Pal, S. *et al.*, *Curr. Sci.*, 1998, **75**, 496-500, (*rev*)