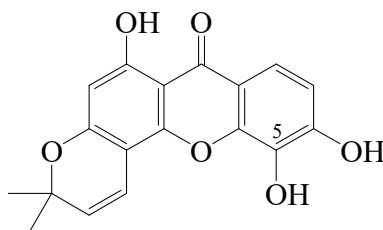




>>Entry Name: Isojacareubin

Synonym(s): 6,10,11-Trihydroxy-3,3-dimethyl-3*H*,7*H*-pyrano[2,3-*c*]xanthen-7-one, 9Cl



CAS Registry Number: 50597-93-8

Molecular Formula: C₁₈H₁₄O₆

Molecular Weight: 326.305

Accurate Mass: 326.07904

Percentage Composition: C 66.26%; H 4.32%; O 29.42%

Biological Source: Constit. of *Hypericum japonicum* and *Hypericum roeperanum*

Physical Description: Yellow needles (MeOH)

Melting Point: Mp 276°

UV: [neutral] λ_{max} 257 (ε 45700); 270 (ε 38900); 302 (ε 17750); 327 (ε 9770); 373 (ε 13490) (MeOH) (Berdy)

>>Derivative: 5-Me ether

Synonym(s): 5-*O*-Methylisojacareubin

CAS Registry Number: 181307-42-6

Molecular Formula: C₁₉H₁₆O₆

Molecular Weight: 340.332

Accurate Mass: 340.09469

Percentage Composition: C 67.05%; H 4.74%; O 28.21%

Biological Source: Constit. of *Hypericum roeperanum*

Physical Description: Yellow gum

Melting Point: Mp 201-205°

UV: [neutral] λ_{max} 251 (log ε 4.15); 319 (log ε 3.67); 367 (log ε 3.6) (MeOH) [neutral] λ_{max} 251 (ε 14125); 319 (ε 4677); 367 (ε 3980) (MeOH) (Berdy) [base] λ_{max} 214 (); 255 (); 263 (); 339 (); 373 () (MeOH-NAOH) (Berdy)

References:

Ishiguro, K. *et al.*, *Phytochemistry*, 1993, **32**, 1583, (*isol, pmr, cryst struct*)

Rath, G. *et al.*, *Phytochemistry*, 1996, **43**, 513, (*5-O-Methylisojacareubin*)