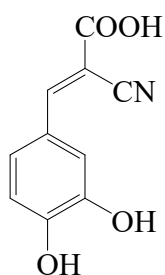




>>Entry Name: 2-Cyano-3-(3,4-dihydroxyphenyl)-2-propenoic acid, 9CI



CAS Registry Number: 118409-56-6

Related CAS Registry Numbers(s): 126716-40-3 126716-52-7 126716-54-9

Molecular Formula: C₁₀H₇NO₄

Molecular Weight: 205.17

Accurate Mass: 205.037509

Percentage Composition: C 58.54%; H 3.44%; N 6.83%; O 31.19%

Melting Point: Mp 240°

>>Variant: (*E*)-form

CAS Registry Number: 122520-79-0

Molecular Formula: C₁₀H₇NO₄

Molecular Weight: 205.17

Accurate Mass: 205.037509

Percentage Composition: C 58.54%; H 3.44%; N 6.83%; O 31.19%

>>Derivative: Et ester

CAS Registry Number: 132464-92-7

Molecular Formula: C₁₂H₁₁NO₄

Molecular Weight: 233.223

Accurate Mass: 233.068809

Percentage Composition: C 61.80%; H 4.75%; N 6.01%; O 27.44%

Biological Use/Importance: Inhibitor of 12– and 15– lipxygenase

>>Derivative: 2-(2-Thienyl)ethyl ester

CAS Registry Number: 132465-10-2

Molecular Formula: C₁₆H₁₃NO₄S

Molecular Weight: 315.349

Accurate Mass: 315.056529

Percentage Composition: C 60.94%; H 4.15%; N 4.44%; O 20.29%; S 10.17%

Biological Use/Importance: Inhibitor of 5-, 12– and 15– lipxygenase

Physical Description: Yellow cryst. (EtOH aq.)

Melting Point: Mp 168-170°

>>Derivative: 3-Phenyl-2-propenyl ester

CAS Registry Number: 132465-11-3

Molecular Formula: C₁₉H₁₅NO₄

Molecular Weight: 321.332

Accurate Mass: 321.100109

Percentage Composition: C 71.02%; H 4.70%; N 4.36%; O 19.92%

Biological Use/Importance: Selective 12– lipxygenase inhibitor

References:

Gazit, A. *et al.*, *J. Med. Chem.*, 1989, **32**, 2344, (*synth*)

Cho, H. *et al.*, *J. Med. Chem.*, 1991, **34**, 1503, (*synth*)

Hussoin, S. *et al.*, *J. Pharm. Sci.*, 1991, **80**, 416, (*pharmacol*)