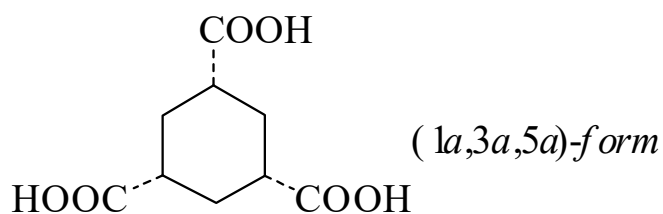




>>Entry Name: 1,3,5-Cyclohexanetricarboxylic acid, 9CI



CAS Registry Number: 25357-95-3

Molecular Formula: C₉H₁₂O₆

Molecular Weight: 216.19

Accurate Mass: 216.06339

Percentage Composition: C 50.00%; H 5.59%; O 44.40%

General Statement: 2 isomers possible, both *meso*-

>>Variant: (1 α ,3 α ,5 α)-form

Synonym(s): *cis*-form

CAS Registry Number: 16526-68-4

Molecular Formula: C₉H₁₂O₆

Molecular Weight: 216.19

Accurate Mass: 216.06339

Percentage Composition: C 50.00%; H 5.59%; O 44.40%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 218-219°

Aldrich: 34434-6

Fluka: 29190

>>Derivative: Tri-Me ester

CAS Registry Number: 6998-83-0

Molecular Formula: C₁₂H₁₈O₆

Molecular Weight: 258.271

Accurate Mass: 258.11034

Percentage Composition: C 55.81%; H 7.02%; O 37.17%

Melting Point: Mp 43-47°

Aldrich: 36229-8

>>Variant: (1 α ,3 α ,5 β)-form

Synonym(s): *trans*-form

CAS Registry Number: 16526-69-5

Molecular Formula: C₉H₁₂O₆

Molecular Weight: 216.19

Accurate Mass: 216.06339

Percentage Composition: C 50.00%; H 5.59%; O 44.40%

Melting Point: Mp 208-210°

References:

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