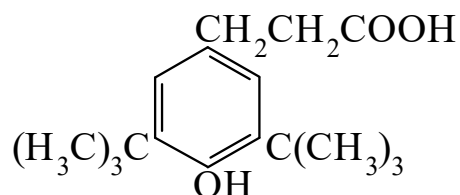




>>Entry Name: 3-(3,5-Di-*tert*-butyl-4-hydroxyphenyl)propanoic acid

Synonym(s): 3,5-Bis(1,1-dimethylethyl)-4-hydroxybenzenepropanoic acid, 9CI. 3,5-Di-*tert*-butyl-4-hydroxyhydrocinnamic acid, 8CI



CAS Registry Number: 20170-32-5

Molecular Formula: C₁₇H₂₆O₃

Molecular Weight: 278.391

Accurate Mass: 278.188195

Percentage Composition: C 73.35%; H 9.41%; O 17.24%

Use/Importance: Esters used as stabilisers and antioxidants in manuf. of polymers

Physical Description: Needles (EtOH aq.) or (C₆H₆/cyclohexane)

Melting Point: Mp 173-175° (172-173°)

Rare Chemicals Library: S4732-6

>>Derivative: Me ester

CAS Registry Number: 6386-38-5

Molecular Formula: C₁₈H₂₈O₃

Molecular Weight: 292.417

Accurate Mass: 292.203845

Percentage Composition: C 73.93%; H 9.65%; O 16.41%

Melting Point: Mp 66-66.5°

>>Derivative: Octadecyl ester

Synonym(s): Irganox 1076. Irganox 1976. Naugard 76

CAS Registry Number: 2082-79-3

Molecular Formula: C₃₅H₆₂O₃

Molecular Weight: 530.873

Accurate Mass: 530.469895

Percentage Composition: C 79.19%; H 11.77%; O 9.04%

Use/Importance: Antioxidant used in manuf. of polymers

Physical Description: Cryst. (MeOH/EtOAc)

Melting Point: Mp 49-50°

Aldrich: 36707-9

>>Derivative: Ester with 1,6-hexanediol (2:1)

Synonym(s): Irganox 249. Irganox 259

CAS Registry Number: 35074-77-2

Molecular Formula: C₄₀H₆₂O₆

Molecular Weight: 638.926

Accurate Mass: 638.45464

Percentage Composition: C 75.19%; H 9.78%; O 15.02%

Use/Importance: Antioxidant for polymers

Physical Description: Off-white powder

Melting Point: Mp 101°

>>Derivative: Ester with diethylene glycol (2:1)

CAS Registry Number: 38879-22-0

Molecular Formula: C₃₈H₅₈O₇

Molecular Weight: 626.872

Accurate Mass: 626.418255

Percentage Composition: C 72.81%; H 9.33%; O 17.87%

Use/Importance: Antioxidant for polymers

Melting Point: Mp 90-91.5°