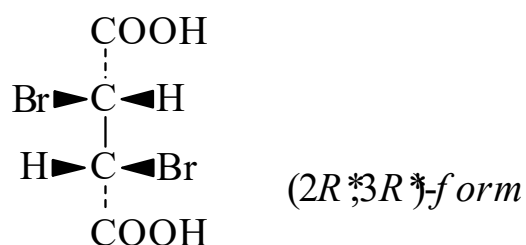




>>Entry Name: 2,3-Dibromobutanedioic acid, 9CI

Synonym(s): 2,3-Dibromosuccinic acid



CAS Registry Number: 526-78-3

Related CAS Registry Numbers(s): 1114-00-7

Molecular Formula: C<sub>4</sub>H<sub>4</sub>Br<sub>2</sub>O<sub>4</sub>

Molecular Weight: 275.881

Accurate Mass: 273.887632

Percentage Composition: C 17.41%; H 1.46%; Br 57.93%; O 23.20%

Rare Chemicals Library: S81996-4

>>Variant: (2R\*,3R\*)-form

Synonym(s): (+)-form

Molecular Formula: C<sub>4</sub>H<sub>4</sub>Br<sub>2</sub>O<sub>4</sub>

Molecular Weight: 275.881

Accurate Mass: 273.887632

Percentage Composition: C 17.41%; H 1.46%; Br 57.93%; O 23.20%

Melting Point: Mp 157-158°

Optical Rotation:  $[\alpha]_D^{24} +147.8$  (EtOAc)

>>Variant: (2S\*,3S\*)-form

Synonym(s): (–)-form

Molecular Formula: C<sub>4</sub>H<sub>4</sub>Br<sub>2</sub>O<sub>4</sub>

Molecular Weight: 275.881

Accurate Mass: 273.887632

Percentage Composition: C 17.41%; H 1.46%; Br 57.93%; O 23.20%

Physical Description: Needles (C<sub>6</sub>H<sub>6</sub>)

Solubility: Sol. H<sub>2</sub>O, MeOH, Me<sub>2</sub>CO, EtOAc; spar. sol. CHCl<sub>3</sub>, petrol

>>Variant: (2RS,3RS)-form

Synonym(s): Isodibromosuccinic acid. Allodibromosuccinic acid

CAS Registry Number: 608-36-6

Molecular Formula: C<sub>4</sub>H<sub>4</sub>Br<sub>2</sub>O<sub>4</sub>

Molecular Weight: 275.881

Accurate Mass: 273.887632

Percentage Composition: C 17.41%; H 1.46%; Br 57.93%; O 23.20%

Melting Point: Mp 166-167°

pKa Value: pK<sub>a1</sub> 1.43; pK<sub>a2</sub> 3.24 (25°)

Aldrich: 10547-3

Fluka: 34020

>>Derivative: Di-Me ester

CAS Registry Number: 1186-98-7

Molecular Formula: C<sub>6</sub>H<sub>8</sub>Br<sub>2</sub>O<sub>4</sub>

Molecular Weight: 303.935

Accurate Mass: 301.918932

Percentage Composition: C 23.71%; H 2.65%; Br 52.58%; O 21.06%

Melting Point: Mp 43°