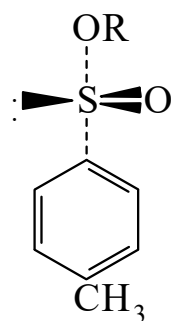




>>Entry Name: 4-Methylbenzenesulfinic acid, 9Cl

Synonym(s): *p*-Toluenesulfinic acid, 8Cl



(*S*)-form of esters

CAS Registry Number: 536-57-2

Related CAS Registry Numbers(s): 824-79-3

Extra CAS Registry Numbers(s): 59153-37-6 64396-66-3 112458-71-6

Molecular Formula: C₇H₈O₂S

Molecular Weight: 156.205

Accurate Mass: 156.0245

Percentage Composition: C 53.82%; H 5.16%; O 20.49%; S 20.53%

Use/Importance: Catalyses double-bond isomerisations and conversion of vinylsilanes to alkenes

Physical Description: Needles (H₂O)

Melting Point: Mp 86-87°

pKa Value: pK_a 1.66 (H₂O)

Rare Chemicals Library: S83549-8

>>Variant: (*S*)-form

Molecular Formula: C₇H₈O₂S

Molecular Weight: 156.205

Accurate Mass: 156.0245

Percentage Composition: C 53.82%; H 5.16%; O 20.49%; S 20.53%

>>Derivative: Me ester

CAS Registry Number: 59203-01-9

Molecular Formula: C₈H₁₀O₂S

Molecular Weight: 170.232

Accurate Mass: 170.04015

Percentage Composition: C 56.45%; H 5.92%; O 18.80%; S 18.84%

Boiling Point: Bp₃ 102-104°

Optical Rotation: [α]_D -201.3 (c, 4.5 in EtOH) (>95% ee)

>>Derivative: Et ester

CAS Registry Number: 59203-02-0

Molecular Formula: C₉H₁₂O₂S

Molecular Weight: 184.259

Accurate Mass: 184.0558

Percentage Composition: C 58.67%; H 6.56%; O 17.37%; S 17.40%

Boiling Point: Bp₃ 105-108°

Optical Rotation: [α]_D -178.8 (EtOH) (85.8% ee)

>>Derivative: (-)-Menthyl ester

Synonym(s): Menthyl 4-methylbenzenesulfinate. Menthyl *p*-toluenesulfinate

CAS Registry Number: 1517-82-4

Molecular Formula: C₁₇H₂₆O₂S

Molecular Weight: 294.457

Accurate Mass: 294.16535

Percentage Composition: C 69.34%; H 8.90%; O 10.87%; S 10.89%

Use/Importance: Reagent used for the Grignard synthesis of optically active sulfoxides

Physical Description: Cryst. (Me₂CO aq.)

Melting Point: Mp 106-107°

Optical Rotation: [α]_D²⁵ -199.2 (c, 2 in Me₂CO)