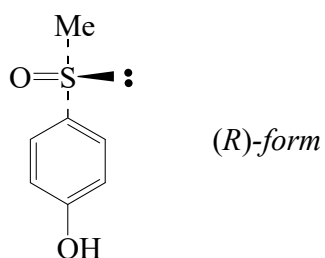




>>Entry Name: 4-(Methylsulfinyl)phenol, 9CI
Synonym(s): *p*-Hydroxyphenyl methyl sulfoxide



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%

>>Variant: (*R*)-form

CAS Registry Number: 93183-65-4
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%
Optical Rotation: [α]_D²⁵+67 (c, 1.0 in Me₂CO) (50% ee)

>>Derivative: Me ether

CAS Registry Number: 93381-75-0
Physical Description: Solid
Optical Rotation: [α]_D²⁰+165.9 (c, 0.38 in CHCl₃) (>95% ee)

>>Variant: (*S*)-form

CAS Registry Number: 158896-00-5
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%
Physical Description: No phys. props. reported

>>Derivative: Me ether

CAS Registry Number: 93381-76-1
Optical Rotation: [α]_D²⁰−102 (c, 2 in CHCl₃) (86% ee)

>>Variant: (±)-form

CAS Registry Number: 14763-64-5
Extra CAS Registry Numbers(s): 158999-84-9
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%
Physical Description: Plates (EtOAc/hexane)
Melting Point: Mp 105-106° (103.5-104°)

>>Derivative: Me ether

Synonym(s): 1-Methoxy-4-(methylsulfinyl)benzene, 9CI. *p*-(Methylsulfinyl)anisole, 8CI

CAS Registry Number: 3517-99-5
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%
Physical Description: Cryst. (petrol)
Melting Point: Mp 45-46° (43°)
Boiling Point: Bp₅ 153-154°. Bp_{0.1} 110-115°

References: