



>>Entry Name: 4-(Methylthio)benzoic acid, 9CI

Synonym(s): 4-Methylmercaptobenzoic acid

CAS Registry Number: 13205-48-6

Molecular Formula: C<sub>8</sub>H<sub>8</sub>O<sub>2</sub>S

Molecular Weight: 168.216

Accurate Mass: 168.0245

Percentage Composition: C 57.12%; H 4.79%; O 19.02%; S 19.06%

Physical Description: Needles (EtOH aq.), leaflets (petrol)

Melting Point: Mp 192°

Aldrich: 14552-1

Fluka: 69326

>>Derivative: Me ester

CAS Registry Number: 3795-79-7

Molecular Formula: C<sub>9</sub>H<sub>10</sub>O<sub>2</sub>S

Molecular Weight: 182.243

Accurate Mass: 182.04015

Percentage Composition: C 59.32%; H 5.53%; O 17.56%; S 17.60%

Melting Point: Mp 82°

>>Derivative: Et ester

CAS Registry Number: 1778-10-5

Molecular Formula: C<sub>10</sub>H<sub>12</sub>O<sub>2</sub>S

Molecular Weight: 196.27

Accurate Mass: 196.0558

Percentage Composition: C 61.20%; H 6.16%; O 16.30%; S 16.34%

Boiling Point: Bp<sub>14</sub> 170°

>>Derivative: Amide

Molecular Formula: C<sub>8</sub>H<sub>9</sub>NOS

Molecular Weight: 167.231

Accurate Mass: 167.040484

Percentage Composition: C 57.46%; H 5.42%; N 8.38%; O 9.57%; S 19.17%

Melting Point: Mp 186°

>>Derivative: Nitrile

CAS Registry Number: 21382-98-9

Molecular Formula: C<sub>8</sub>H<sub>7</sub>NS

Molecular Weight: 149.216

Accurate Mass: 149.029919

Percentage Composition: C 64.40%; H 4.73%; N 9.39%; S 21.49%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 64°

Boiling Point: Bp 272°

Aldrich: 27968-4

>>Derivative: S,S-Dioxide

Synonym(s): 4-(Methylsulfonyl)benzoic acid, 9CI

CAS Registry Number: 4052-30-6

Physical Description: Cryst.

Melting Point: Mp 274-276°

Aldrich: 13641-7

>>Derivative: S,S-Dioxide, Me ester