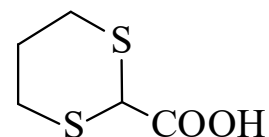




>>Entry Name: 1,3-Dithiane-2-carboxylic acid, 9CI



CAS Registry Number: 20461-89-6

Molecular Formula: C<sub>5</sub>H<sub>8</sub>O<sub>2</sub>S<sub>2</sub>

Molecular Weight: 164.249

Accurate Mass: 163.99657

Percentage Composition: C 36.56%; H 4.91%; O 19.48%; S 39.05%

Physical Description: Pale yellow cryst. (C<sub>6</sub>H<sub>6</sub>/pentane)

Melting Point: Mp 115-116°

>>Derivative: Me ester

CAS Registry Number: 56579-84-1

Molecular Formula: C<sub>6</sub>H<sub>10</sub>O<sub>2</sub>S<sub>2</sub>

Molecular Weight: 178.276

Accurate Mass: 178.01222

Percentage Composition: C 40.42%; H 5.65%; O 17.95%; S 35.97%

Melting Point: Mp 28°

>>Derivative: Et ester

Synonym(s): Ethyl 1,3-dithiane-2-carboxylate

CAS Registry Number: 20462-00-4

Molecular Formula: C<sub>7</sub>H<sub>12</sub>O<sub>2</sub>S<sub>2</sub>

Molecular Weight: 192.303

Accurate Mass: 192.02787

Percentage Composition: C 43.72%; H 6.29%; O 16.64%; S 33.35%

Use/Importance: Reagent for synth. of α-ketoesters

Boiling Point: Bp<sub>0.2</sub> 75-77°

Aldrich: 23541-5

Fluka: 43749

>>Derivative: Et ester, 1,3-dioxide(1*R*,3*R*-)

Molecular Formula: C<sub>7</sub>H<sub>12</sub>O<sub>4</sub>S<sub>2</sub>

Molecular Weight: 224.301

Accurate Mass: 224.0177

Percentage Composition: C 37.48%; H 5.39%; O 28.53%; S 28.59%

Physical Description: Cryst. solid (EtOAc)

Melting Point: Mp 132-133°

Optical Rotation: [α]<sub>D</sub> +240 (c, 3 in CHCl<sub>3</sub>) (ee >97%)

>>Derivative: Et ester, 1,3-dioxide(1*RS*,3*RS*-)

Molecular Formula: C<sub>7</sub>H<sub>12</sub>O<sub>4</sub>S<sub>2</sub>

Molecular Weight: 224.301

Accurate Mass: 224.0177

Percentage Composition: C 37.48%; H 5.39%; O 28.53%; S 28.59%

Physical Description: Cryst. (*tert*-butyl acetate)

Melting Point: Mp 108-112°

>>Derivative: Benzyl ester

CAS Registry Number: 64114-00-7

Molecular Formula: C<sub>12</sub>H<sub>14</sub>O<sub>2</sub>S<sub>2</sub>

Molecular Weight: 254.373

Accurate Mass: 254.04352

Percentage Composition: C 56.66%; H 5.55%; O 12.58%; S 25.21%

Physical Description: Cryst. (hexane)

Melting Point: Mp 72-75°