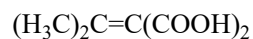




>>Entry Name: (1-Methylethylidene)propanedioic acid, 9CI

Synonym(s): Isopropylidenemalonic acid



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

Molecular Weight: 144.127

Accurate Mass: 144.04226

Percentage Composition: C 50.00%; H 5.59%; O 44.40%

>>Derivative: Di-Me ester

CAS Registry Number: 22035-53-6

Molecular Formula: C<sub>8</sub>H<sub>12</sub>O<sub>4</sub>

Molecular Weight: 172.18

Accurate Mass: 172.07356

Percentage Composition: C 55.81%; H 7.02%; O 37.17%

Boiling Point: Bp<sub>18</sub> 116°

>>Derivative: Di-Et ester

CAS Registry Number: 6802-75-1

Molecular Formula: C<sub>10</sub>H<sub>16</sub>O<sub>4</sub>

Molecular Weight: 200.234

Accurate Mass: 200.10486

Percentage Composition: C 59.98%; H 8.05%; O 31.96%

Boiling Point: Bp<sub>10</sub> 110-115°

Aldrich: 27803-3

Fluka: 59536

Rare Chemicals Library: S3893-9

Sigma: I5388

>>Derivative: Mononitrile

>>Derivative: Nitrile, Me ester

Synonym(s): Methyl 2-cyano-3-methyl-2-butenolate, 9CI

CAS Registry Number: 6666-75-7

Molecular Formula: C<sub>7</sub>H<sub>9</sub>NO<sub>2</sub>

Molecular Weight: 139.154

Accurate Mass: 139.063329

Percentage Composition: C 60.42%; H 6.52%; N 10.07%; O 23.00%

Boiling Point: Bp<sub>3</sub> 97°

Rare Chemicals Library: S35278-0

>>Derivative: Dinitrile

Synonym(s): (1-Methylethylidene)propanedinitrile, 9CI. Isopropylidenemalononitrile. 1,1-Dicyano-2-methylpropene

CAS Registry Number: 13166-10-4

Molecular Formula: C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>

Molecular Weight: 106.127

Accurate Mass: 106.053098

Percentage Composition: C 67.91%; H 5.70%; N 26.40%

Boiling Point: Bp<sub>23</sub> 108°

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Mirek, J. *et al.*, *Synthesis*, 1980, 296, (*dinitrile*)  
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Chen, Y.L. *et al.*, *J. Med. Chem.*, 1997, **40**, 1749-1754, (*dinitrile*)