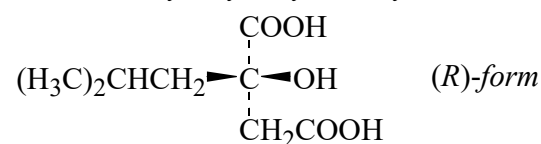




>>Entry Name: 2-Hydroxy-2-(2-methylpropyl)butanedioic acid

Synonym(s): 2-Hydroxy-5-methylhexane-1,2-dicarboxylic acid. 3-Carboxy-3-hydroxy-5-methylhexanoic acid. 2-Isobutylmalic acid



CAS Registry Number: 60924-65-4

Related CAS Registry Numbers(s): 51692-86-5 58139-24-5

Extra CAS Registry Numbers(s): 51692-87-6

Molecular Formula: C<sub>8</sub>H<sub>14</sub>O<sub>5</sub>

Molecular Weight: 190.196

Accurate Mass: 190.084125

Percentage Composition: C 50.52%; H 7.42%; O 42.06%

>>Variant: (R)-form

CAS Registry Number: 51692-95-6

Molecular Formula: C<sub>8</sub>H<sub>14</sub>O<sub>5</sub>

Molecular Weight: 190.196

Accurate Mass: 190.084125

Percentage Composition: C 50.52%; H 7.42%; O 42.06%

Biological Source: Constit. of the roots of *Dactylorhiza hatagirea*

Physical Description: Needles

Melting Point: Mp 161-162°

Optical Rotation: [α]<sub>D</sub> −8.4 (c, 0.51 in MeOH)

>>Derivative: O-β-D-Glucopyranoside

Synonym(s): Dactylorhin C

CAS Registry Number: 256459-23-1

Molecular Formula: C<sub>14</sub>H<sub>24</sub>O<sub>10</sub>

Molecular Weight: 352.338

Accurate Mass: 352.13695

Percentage Composition: C 47.73%; H 6.87%; O 45.41%

Biological Source: Constit. of the roots of *Dactylorhiza hatagirea*

Physical Description: Amorph. powder

Optical Rotation: [α]<sub>D</sub><sup>24</sup> −24 (c, 1.15 in MeOH)

>>Derivative: Bis(4-β-D-glucopyranosyloxybenzyl) ester

Synonym(s): Militarine

CAS Registry Number: 58139-23-4

Molecular Formula: C<sub>34</sub>H<sub>46</sub>O<sub>17</sub>

Molecular Weight: 726.727

Accurate Mass: 726.273505

Percentage Composition: C 56.19%; H 6.38%; O 37.43%

Source/Synthesis: Constit. of *Orchis militaris* and *Dactylorhiza hatagirea*

Physical Description: Amorph. solid

Optical Rotation: [α]<sub>D</sub><sup>25</sup> −47 (c, 0.78 in MeOH)

>>Derivative: O-β-D-Glucopyranoside, 1-(4-β-D-glucopyranosyloxybenzyl) ester,

Synonym(s): Dactylorhin E

CAS Registry Number: 256459-40-2

Molecular Formula: C<sub>27</sub>H<sub>40</sub>O<sub>16</sub>

Molecular Weight: 620.603

Accurate Mass: 620.23164

Percentage Composition: C 52.26%; H 6.50%; O 41.25%

Biological Source: Constit. of the roots of *Dactylorhiza hatagirea*

Physical Description: Amorph. powder

Optical Rotation: [α]<sub>D</sub><sup>25</sup> −39.7 (c, 0.73 in MeOH)

UV: [neutral] λ<sub>max</sub> 223 (log ε 3.94); 271 (log ε 2.89); 277 (log ε 2.82) (MeOH)