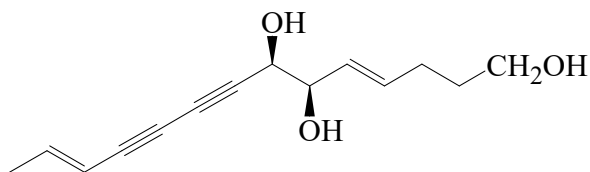




>>Entry Name: 4,12-Tetradecadiene-8,10-diyne-1,6,7-triol, 9CI

Synonym(s): Lobetyol



CAS Registry Number: 136171-87-4

Related CAS Registry Numbers(s): 40111-24-8 136033-43-7

Molecular Formula: C<sub>14</sub>H<sub>18</sub>O<sub>3</sub>

Molecular Weight: 234.294

Accurate Mass: 234.125595

Percentage Composition: C 71.77%; H 7.74%; O 20.49%

Biological Source: Isol. from the hairy roots of *Lobelia inflata* and *Campanula* spp.

Physical Description: Off-white amorph. powder

Optical Rotation:  $[\alpha]_D^{26} +18.8$  (c, 0.13 in Me<sub>2</sub>CO).  $[\alpha]_D^{20} +33$  (c, 0.745 in EtOH)

>>Derivative: Tri-Ac

CAS Registry Number: 136033-43-7

Molecular Formula: C<sub>20</sub>H<sub>24</sub>O<sub>6</sub>

Molecular Weight: 360.406

Accurate Mass: 360.15729

Percentage Composition: C 66.65%; H 6.71%; O 26.64%

Physical Description: Off-white amorph. powder

Optical Rotation:  $[\alpha]_D^{26} -79.2$  (c, 0.28 in CHCl<sub>3</sub>)

>>Derivative: 6-O-β-D-Glucopyranoside

Synonym(s): Lobetyolin

CAS Registry Number: 136085-37-5

Molecular Formula: C<sub>20</sub>H<sub>28</sub>O<sub>8</sub>

Molecular Weight: 396.436

Accurate Mass: 396.17842

Percentage Composition: C 60.59%; H 7.12%; O 32.29%

Biological Source: Isol. from the hairy roots of *Lobelia inflata*

Physical Description: Off-white amorph. powder

Optical Rotation:  $[\alpha]_D^{28} -8.9$  (c, 0.12 in Me<sub>2</sub>CO)

>>Derivative: 6-O-β-D-Glucopyranoside, hexa-Ac

CAS Registry Number: 136005-81-7

Physical Description: Off-white amorph. powder

Optical Rotation:  $[\alpha]_D^{26} -71.4$  (c, 0.55 in CHCl<sub>3</sub>)

>>Derivative: 6-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]

Synonym(s): Lobetyolinin

CAS Registry Number: 142451-48-7

Molecular Formula: C<sub>26</sub>H<sub>38</sub>O<sub>13</sub>

Molecular Weight: 558.578

Accurate Mass: 558.231245

Percentage Composition: C 55.91%; H 6.86%; O 37.24%

Biological Source: Isol. from the hairy roots of *Lobelia inflata*

Physical Description: Off-white amorph. powder

Optical Rotation:  $[\alpha]_D^{30} -41.7$  (c, 0.59 in MeOH)