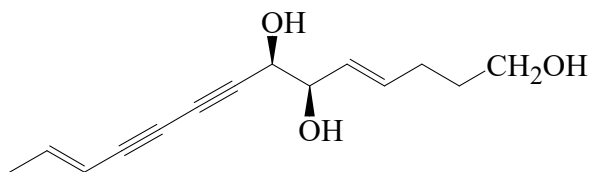




>>Entry Name: 4,12-Tetradecadiene-8,10-diyne-1,6,7-triol, 9CI

Synonym(s): Lobetyol



CAS Registry Number: 136171-87-4

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

Molecular Formula: $C_{14}H_{18}O_3$

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_2CO). $[\alpha]_D^{20} +33$ (c, 0.745 in EtOH)

>>Derivative: Tri-Ac

CAS Registry Number: 136033-43-7

Molecular Formula: $C_{20}H_{24}O_6$

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 $CHCl_3$)

>>Derivative: 6-O- β -D-Glucopyranoside

Synonym(s): Lobetyolin

CAS Registry Number: 136085-37-5

Molecular Formula: $C_{20}H_{28}O_8$

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_2CO)

>>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 $CHCl_3$)

>>Derivative: 6-O-[β -D-Glucopyranosyl-(1 $\rightarrow$ 6)- β -D-glucopyranoside]

Synonym(s): Lobetyolinin

CAS Registry Number: 142451-48-7

Molecular Formula: $C_{26}H_{38}O_{13}$

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)