



Accurate Mass: 344.12599
Percentage Composition: C 66.27%; H 5.85%; O 27.88%
Biological Source: Constit. of *Lithospermum erythrorhizon*
Biological Use/Importance: Exhibits antifungal, antiviral and cytotoxic props.

>>Derivative: O^I -(2-Methylpropanoyl)
Synonym(s): Isobutyrylshikonin. Shikonin isobutyrate

CAS Registry Number: 52438-12-7

Molecular Formula: $C_{20}H_{22}O_6$
Molecular Weight: 358.39
Accurate Mass: 358.14164
Percentage Composition: C 67.03%; H 6.19%; O 26.79%
Biological Source: Isol. from roots of *Lithospermum erythrorhizon*
Melting Point: Mp 89-90°
Optical Rotation: $[\alpha]_{600}^{23} +125$ (EtOH)

>>Derivative: O^I -(2-Methylbutanoyl)
Synonym(s): α -Methylbutyrylshikonin

CAS Registry Number: 52387-15-2

Molecular Formula: $C_{21}H_{24}O_6$
Molecular Weight: 372.417
Accurate Mass: 372.15729
Percentage Composition: C 67.73%; H 6.50%; O 25.78%
Biological Source: Constit. of *Lithospermum erythrorhizon* and other plant spp.

>>Derivative: O^I -(3-Methylbutanoyl)
Synonym(s): Isovalerylshikonin

CAS Registry Number: 52387-14-1

Molecular Formula: $C_{21}H_{24}O_6$
Molecular Weight: 372.417
Accurate Mass: 372.15729
Percentage Composition: C 67.73%; H 6.50%; O 25.78%
Biological Source: Constit. of *Lithospermum* spp. and *Macrotomia euchroma*

>>Derivative: O^I -(3-Hydroxy-3-methylbutanoyl)
Synonym(s): β -Hydroxyisovalerylshikonin

CAS Registry Number: 7415-78-3

Molecular Formula: $C_{21}H_{24}O_7$
Molecular Weight: 388.416
Accurate Mass: 388.152205
Percentage Composition: C 64.94%; H 6.23%; O 28.83%
Biological Source: Isol. from *Lithospermum erythrorhizon* and *Lithospermum euchromum*
Physical Description: Red-violet cryst.
Melting Point: Mp 90-92°
Optical Rotation: $[\alpha]_{600}^{15} +128$ (EtOH)

>>Derivative: O^I -(3-Acetoxy-3-methylbutanoyl)
Synonym(s): β -Acetoxyisovalerylshikonin

CAS Registry Number: 98936-77-7

Molecular Formula: $C_{23}H_{26}O_8$
Molecular Weight: 430.454
Accurate Mass: 430.16277
Percentage Composition: C 64.18%; H 6.09%; O 29.73%
Biological Source: Constit. of *Macrotomia euchroma*