



Physical Description: Cryst. (EtOH)

Melting Point: Mp 168°

>>**Derivative:** 1-(3-Methylthio-2Z-propenoyl), 9-Ac

Synonym(s): Bakkenolide D, S-Fukinolide

CAS Registry Number: 18456-03-6

Molecular Formula: C₂₁H₂₈O₆S

Molecular Weight: 408.515

Accurate Mass: 408.16066

Percentage Composition: C 61.74%; H 6.91%; O 23.50%; S 7.85%

Biological Source: Constit. of *Petasites japonicus*

Physical Description: Cryst. (petrol)

Melting Point: Mp 200-201°

Optical Rotation: [α]_D²² -161 (c, 1 in CHCl₃)

>>**Derivative:** 9-(3-Methylthio-2Z-propenoyl), 1-Ac

Synonym(s): Bakkenolide D_d

CAS Registry Number: 226711-25-7

Molecular Formula: C₂₁H₂₈O₆S

Molecular Weight: 408.515

Accurate Mass: 408.16066

Percentage Composition: C 61.74%; H 6.91%; O 23.50%; S 7.85%

Biological Source: Constit. of *Petasites formosanus*

Physical Description: Oil

Optical Rotation: [α]_D -103 (c, 0.031 in MeOH)

UV: [neutral] $\lambda_{\max}$ 290 (log ϵ 3.68) (MeOH)

>>**Derivative:** 1-(3-Methylsulfinyl-2-propenoyl)

Synonym(s): Bakkenolide Y_b

CAS Registry Number: 226711-51-9

Molecular Formula: C₁₉H₂₆O₆S

Molecular Weight: 382.477

Accurate Mass: 382.14501

Percentage Composition: C 59.67%; H 6.85%; O 25.10%; S 8.38%

Biological Source: Constit. of *Petasites formosanus*

>>**Derivative:** 1-(3-Methylsulfinyl-2-propenoyl)(R,Z-), 9-Ac

Synonym(s): Bakkenolide D_b

CAS Registry Number: 226711-23-5

Molecular Formula: C₂₁H₂₈O₇S

Molecular Weight: 424.514

Accurate Mass: 424.155575

Percentage Composition: C 59.42%; H 6.65%; O 26.38%; S 7.55%

Biological Source: Constit. of *Petasites formosanus*

Physical Description: Oil

Optical Rotation: [α]_D -72 (c, 0.2 in MeOH)

UV: [neutral] $\lambda_{\max}$ 286 (log ϵ 3.09) (MeOH)