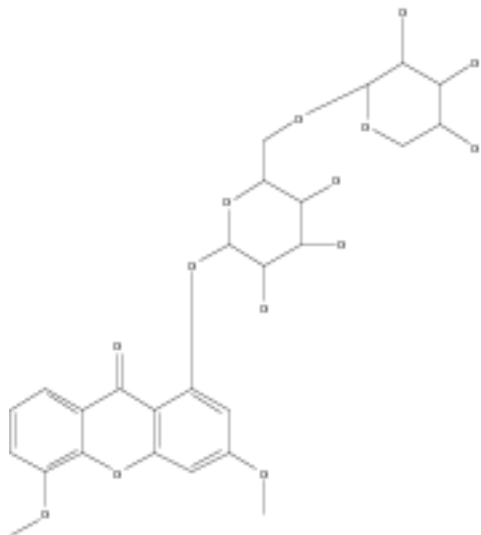


Task History

Task Began February 26, 2021 02:25 AM

Explore substances by SIMILARITY\_2D\_EXACT



Candidates: 9

**Candidates Selected (ID 4)**

99 (most similar)

Answer Type: Substances

Result Count: 1

**Detailed display**

From ID: 4

Type: 119737-00-7

CAS Registry Number: 119737-00-7

C<sub>26</sub> H<sub>30</sub> O<sub>14</sub>

9*H*-Xanthen-9-one, 3,5-dimethoxy-1-[(6-*O*-β-D-xylopyranosyl-β-D-glucopyranosyl)oxy]-

**Molecular Weight**

566.51

**Boiling Point (Predicted)**

Value: 879.4±65.0 °C | Condition: Press: 760 Torr

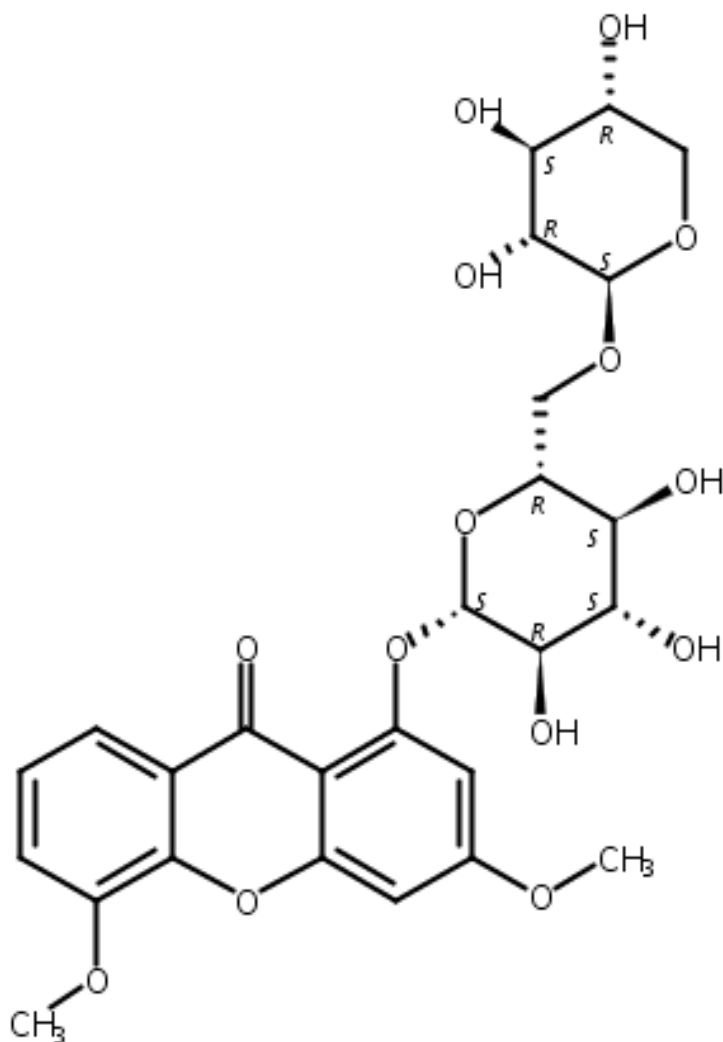
**Density (Predicted)**

Value: 1.63±0.1 g/cm<sup>3</sup> | Condition: Temp: 20 °C Press: 760 Torr

**pKa (Predicted)**

Value: 12.62±0.70 | Condition: Most Acidic Temp: 25 °C

**Other Names:** 3,5-Dimethoxy-1-[(6-*O*-β-D-xylopyranosyl-β-D-glucopyranosyl)oxy]-9*H*-xanthen-9-one



Absolute stereochemistry.

~10 References

**Experimental Properties:** Spectra

Spectra Properties	Value	Condition	Note
Carbon-13 NMR Spectrum	See spectrum		(1)WSS

(1) WSS: Wolfgang Robien / University of Vienna (Spectral Data were obtained from Wiley Subscription Services, Inc. (US))

**Predicted Properties:** Biological Chemical Density Lipinski Spectra Structure Related Thermal

<b>Biological Properties</b>	<b>Value</b>	<b>Condition</b>	<b>Note</b>
Bioconcentration Factor	1.0	pH 1 Temp: 25 °C	(2)
Bioconcentration Factor	1.0	pH 2 Temp: 25 °C	(2)
Bioconcentration Factor	1.0	pH 3 Temp: 25 °C	(2)
Bioconcentration Factor	1.0	pH 4 Temp: 25 °C	(2)
Bioconcentration Factor	1.0	pH 5 Temp: 25 °C	(2)
Bioconcentration Factor	1.0	pH 6 Temp: 25 °C	(2)
Bioconcentration Factor	1.0	pH 7 Temp: 25 °C	(2)
Bioconcentration Factor	1.0	pH 8 Temp: 25 °C	(2)
Bioconcentration Factor	1.0	pH 9 Temp: 25 °C	(2)
Bioconcentration Factor	1.0	pH 10 Temp: 25 °C	(2)
<b>Chemical Properties</b>	<b>Value</b>	<b>Condition</b>	<b>Note</b>
Koc	9.02	pH 1 Temp: 25 °C	(2)
Koc	9.02	pH 2 Temp: 25 °C	(2)
Koc	9.02	pH 3 Temp: 25 °C	(2)
Koc	9.02	pH 4 Temp: 25 °C	(2)
Koc	9.02	pH 5 Temp: 25 °C	(2)
Koc	9.02	pH 6 Temp: 25 °C	(2)
Koc	9.02	pH 7 Temp: 25 °C	(2)
Koc	9.02	pH 8 Temp: 25 °C	(2)
Koc	9.01	pH 9 Temp: 25 °C	(2)
Koc	8.96	pH 10 Temp: 25 °C	(2)
logD	-0.78	pH 1 Temp: 25 °C	(2)
logD	-0.78	pH 2 Temp: 25 °C	(2)
logD	-0.78	pH 3 Temp: 25 °C	(2)
logD	-0.78	pH 4 Temp: 25 °C	(2)
logD	-0.78	pH 5 Temp: 25 °C	(2)
logD	-0.78	pH 6 Temp: 25 °C	(2)
logD	-0.78	pH 7 Temp: 25 °C	(2)
logD	-0.78	pH 8 Temp: 25 °C	(2)
logD	-0.78	pH 9 Temp: 25 °C	(2)
logD	-0.78	pH 10 Temp: 25 °C	(2)
logP	-0.775±0.800	Temp: 25 °C	(2)
Mass Intrinsic Solubility	Sparingly Soluble (1.8E-3 g/L)	Temp: 25 °C	(2)
Mass Solubility	Sparingly Soluble (1.8E-3 g/L)	pH 1 Temp: 25 °C	(2)
Mass Solubility	Sparingly Soluble (1.8E-3 g/L)	pH 2 Temp: 25 °C	(2)
Mass Solubility	Sparingly Soluble (1.8E-3 g/L)	pH 3 Temp: 25 °C	(2)
Mass Solubility	Sparingly Soluble (1.8E-3 g/L)	pH 4 Temp: 25 °C	(2)
Mass Solubility	Sparingly Soluble (1.8E-3 g/L)	pH 5 Temp: 25 °C	(2)
Mass Solubility	Sparingly Soluble (1.8E-3 g/L)	pH 6 Temp: 25 °C	(2)
Mass Solubility	Sparingly Soluble (1.8E-3 g/L)	pH 7 Temp: 25 °C	(2)
Mass Solubility	Sparingly Soluble (1.8E-3 g/L)	pH 8 Temp: 25 °C	(2)
Mass Solubility	Sparingly Soluble (1.8E-3 g/L)	pH 9 Temp: 25 °C	(2)
Mass Solubility	Sparingly Soluble (1.8E-3 g/L)	pH 10 Temp: 25 °C	(2)
Mass Solubility	Sparingly Soluble (1.8E-3 g/L)	Unbuffered Water pH 7.00 Temp: 25 °C	(2)
Molar Intrinsic Solubility	Sparingly Soluble (3.2E-6 mol/L)	Temp: 25 °C	(2)
Molar Solubility	Sparingly Soluble (3.2E-6 mol/L)	pH 1 Temp: 25 °C	(2)
Molar Solubility	Sparingly Soluble (3.2E-6 mol/L)	pH 2 Temp: 25 °C	(2)
Molar Solubility	Sparingly Soluble (3.2E-6 mol/L)	pH 3 Temp: 25 °C	(2)
Molar Solubility	Sparingly Soluble (3.2E-6 mol/L)	pH 4 Temp: 25 °C	(2)
Molar Solubility	Sparingly Soluble (3.2E-6 mol/L)	pH 5 Temp: 25 °C	(2)
Molar Solubility	Sparingly Soluble (3.2E-6 mol/L)	pH 6 Temp: 25 °C	(2)
Molar Solubility	Sparingly Soluble (3.2E-6 mol/L)	pH 7 Temp: 25 °C	(2)
Molar Solubility	Sparingly Soluble (3.2E-6 mol/L)	pH 8 Temp: 25 °C	(2)
Molar Solubility	Sparingly Soluble (3.2E-6 mol/L)	pH 9 Temp: 25 °C	(2)
Molar Solubility	Sparingly Soluble (3.2E-6 mol/L)	pH 10 Temp: 25 °C	(2)

Molar Solubility	Sparingly Soluble (3.2E-6 mol/L)	Unbuffered Water pH 7.00 Temp: 25 °C	(2)
Molecular Weight	566.51		(2)
pKa	12.62±0.70	Most Acidic Temp: 25 °C	(2)
Vapor Pressure	4.15E-33 Torr	Temp: 25 °C	(2)
<b>Density Properties</b>	<b>Value</b>	<b>Condition</b>	<b>Note</b>
Density	1.63±0.1 g/cm3	Temp: 20 °C Press: 760 Torr	(2)
Molar Volume	347.5±5.0 cm3/mol	Temp: 20 °C Press: 760 Torr	(2)
<b>Lipinski Properties</b>	<b>Value</b>	<b>Condition</b>	<b>Note</b>
Freely Rotatable Bonds	13		(2)
H Acceptors	14		(2)
H Donors	6		(2)
H Donor/Acceptor Sum	20		(2)
logP	-0.775±0.800	Temp: 25 °C	(2)
Molecular Weight	566.51		(2)
<b>Structure Related Properties</b>	<b>Value</b>	<b>Condition</b>	<b>Note</b>
Polar Surface Area	203 A2		(2)
<b>Thermal Properties</b>	<b>Value</b>	<b>Condition</b>	<b>Note</b>
Boiling Point	879.4±65.0 °C	Press: 760 Torr	(2)
Enthalpy of Vaporization	133.90±3.0 kJ/mol	Press: 760 Torr	(2)
Flash Point	294.7±27.8 °C		(2)
<b>Spectra Properties</b>	<b>Value</b>	<b>Condition</b>	<b>Note</b>
Carbon-13 NMR Spectrum	See spectrum		(3)
Proton NMR Spectrum	See spectrum		(3)

(2) Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2021 ACD/Labs)

(3) Predicted NMR data calculated using Advanced Chemistry Development, Inc. (ACD/Labs) Software V11.01 (© 1994-2021 ACD/Labs)

CAS Role	Patents	Nonpatents	Nonspecific Derivatives from Patents	Nonspecific Derivatives from Nonpatents
Analytical Study		✓		
Biological Study		✓		
Occurrence		✓		
Preparation		✓		
Process		✓		
Properties		✓		
Uses		✓		

**Document Type(s):** Journal

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