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Typical Product Specifications & Properties

thonningianin A

CAS Number: : 271579-11-4

Specifications	Limits
Canonicalized Compound	1
Compound Complexity	1590
Hydrogen Bond Acceptor Count	21
Hydrogen Bond Donor Count	12
Rotatable Bond Count	9
Allowed IUPAC Name	[(10R,11R,12R,13S,15R)-13-[3,5-dihydroxy-4-(3-phenylpropanoyl)phenoxy]-3,4,5,12,21,22,23-heptahydroxy-8,18-dioxo-9,14,17-trioxatetracyclo[17.4.0.02,7.010,15]tricosan-1(23),2,4,6,19,21-hexaen-11-yl] 3,4,5-trihydroxybenzoate
CAS-like Style IUPAC Name	3,4,5-trihydroxybenzoic acid [(10R,11R,12R,13S,15R)-13-[3,5-dihydroxy-4-(1-oxo-3-phenylpropyl)phenoxy]-3,4,5,12,21,22,23-heptahydroxy-8,18-dioxo-9,14,17-trioxatetracyclo[17.4.0.02,7.010,15]tricosan-1(23),2,4,6,19,21-hexaen-11-yl] ester
Markup IUPAC Name	[(10<I>R</I>,11<I>R</I>,12<I>R</I>,13<I>S</I>,15<I>R</I>)-13-[3,5-dihydroxy-4-(3-phenylpropanoyl)phenoxy]-3,4,5,12,21,22,23-heptahydroxy-8,18-dioxo-9,14,17-trioxatetracyclo[17.4.0.0^{2,7}.0^{10,15}]tricosan-1(23),2,4,6,19,21-hexaen-11-yl] 3,4,5-trihydroxybenzoate
Preferred IUPAC Name	[(10R,11R,12R,13S,15R)-13-[3,5-dihydroxy-4-(3-phenylpropanoyl)phenoxy]-3,4,5,12,21,22,23-heptahydroxy-8,18-dioxo-9,14,17-trioxatetracyclo[17.4.0.02,7.010,15]tricosan-1(23),2,4,6,19,21-hexaen-11-yl] 3,4,5-trihydroxybenzoate
Systematic IUPAC Name	[(10R,11R,12R,13S,15R)-13-[3,5-bis(oxidanyl)-4-(3-phenylpropanoyl)phenoxy]-3,4,5,12,21,22,23-heptakis(oxidanyl)-9,14,17-trioxatetracyclo[17.4.0.02,7.010,15]tricosan-1(23),2,4,6,19,21-hexaen-11-yl] 3,4,5-tris(oxidanyl)benzoate

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Systematic
IUPAC Name

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Traditional
IUPAC Name

Standard
InChI

3,4,5-trihydroxybenzoic acid [(10R,11R,12R,13S,15R)-13-(4-hydrocinnamoyl-3,5-dihydroxy-phenoxy)-3,4,5,12,21,22,23-heptahydroxy-8,18-diketo-9,14,17-trioxatetracyclo[17.4.0.02,7.010,15]tricoso-1(23),2,4,6,19,21-hexa-11-yl] ester

InChI=1S/C42H34O21/c43-20(7-6-15-4-2-1-3-5-15)30-21(44)10-22(30)45)60-42-36(55)38(63-39(56)16-8-23(46)31(50)24(47)9-127(61-42)14-59-40(57)18-12-25(48)32(51)34(53)28(18)29-19(41)37)13-26(49)33(52)35(29)54/h1-5,8-13,27,36-38,42,44-55H,6-7,14H2/t27-,36-,37-,38-,42-/m1/s1

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Specifications	Limits
Standard	XQVKQEFQGYTUAR-VHBRHXFYSA-N
Specifications	Limits

InChIKey

XLogP3-AA
Log P

3.8

Exact Mass

874.15925809

Molecular

874.7

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Weight
Canonical
SMILES

Isomeric
SMILES

Polar Surface
Area
Topological

Monoisotopic
Weight

374.7
C1C2C(C(C(C(O2)OC3=CC(=C(C(=C3)O)C(=O)CCC4=CC=CC=C4)O)O)OC3=CC(=C(C(=C3)O)C(=O)CCC4=CC=CC=C4)O)O)O

357

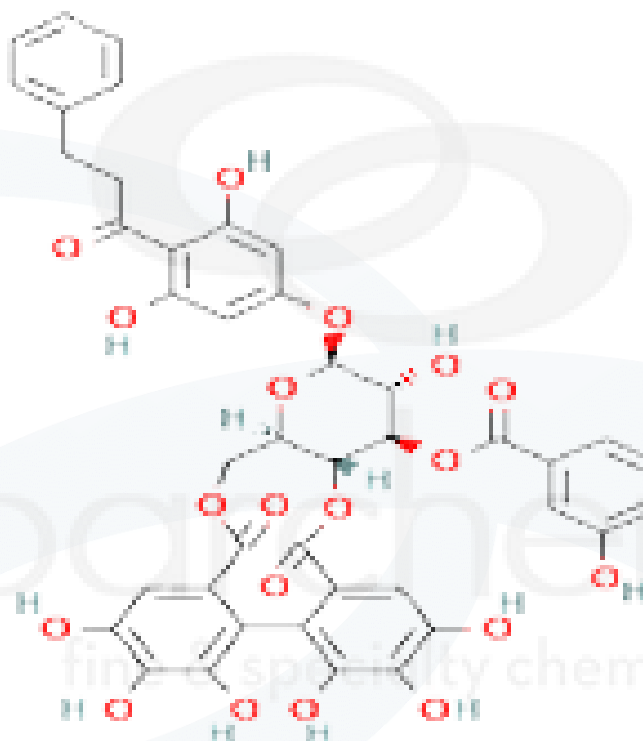
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