Typical Product Specifications & Properties

thonningianin A

CAS Number: : 271579-11-4

Specifications	Limits
Molecular Formula	C42H34O21
Molecular weight	
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]tricosa-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]tricosa-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}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]tricosa-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(oxidanbis(oxidanylidene)-9,14,17-trioxatetracyclo[17.4.0.02,7.010,15]tricosa-1(23),2,4,6,19,21-he11-yl] 3,4,5-tris(oxidanyl)benzoate

Specifications	Limits
Traditional IUPAC Name	3,4,5-trihydroxybenzoic acid [(10R,11R,12R,13S,15R)-13-(4-hydro trioxatetracyclo[17.4.0.02,7.010,15]tricosa-1(23),2,4,6,19,21-hex
Standard InChI	InChI=1S/C42H34O21/c43-20(7-6-15-4-2-1-3-5-15)30-21(44)10-1 25(48)32(51)34(53)28(18)29-19(41(58)62-37)13-26(49)33(52)35
Standard InChIKey	XQVKQEFQGYTUAR-VHBRHXFYSA-N

Specifications	Limits
XLogP3-AA Log P	3.8
Exact Mass	874.15925809
Molecular Weight	874.7

Canonical SMILES	C1C2C(C(C(O2)OC3=CC(=C(C(=C3)O)C(=O)CCC4=CC=C
Isomeric SMILES	C1[C@@H]2[C@H]([C@@H]([C@H]([C@@H](O2)OC3=CC(=C(C(=C3)O)C(=O)CCC4=CC=CC=C4O)O)O)O
Polar Surface Area Topological	357
Monoisotopic Weight	874.15925809
Chemical Structure	chemicalStructure-thonningianin-a