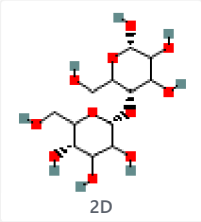
Case No.: IPR2023-00206
U.S. Patent No. 9,943,096

PubChem

COMPOUND SUMMARY

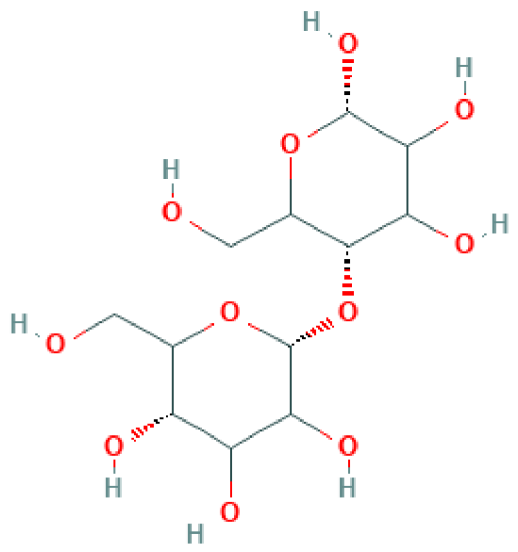
Maltodextrin-dextrose equivalent 10-15

PubChem CID	68229136
Structure	 2D Find Similar Structures
Molecular Formula	$C_{12}H_{22}O_{11}$
Synonyms	SCHEMBL12278702 Maltodextrin - dextrose equivalent 10-15
Molecular Weight	342.30
Dates	Modify 2022-11-12 Create 2012-11-30

1 Structures

1.1 2D Structure

Chemical Structure Depiction



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1.2 3D Status

Conformer generation is disallowed since too many undefined stereo centers

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2 Biologic Description

SVG Image	
IUPAC Condensed	Hex(?1-4)Hex
LINUCS	[]\[Hexp]{[(4+1)]\[Hexp]{}}
IUPAC	hexopyranosyl-(1->4)-hexopyranose
WURCS	WURCS=2.0/1,2,1/[axx2xh-1x_1-5]/1-1/a4-b1

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3 Names and Identifiers

3.1 Computed Descriptors

3.1.1 IUPAC Name

(3*S*,6*R*)-2-(hydroxymethyl)-6-[(3*S*,6*S*)-4,5,6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxyoxane-3,4,5-triol

Computed by LexiChem 2.6.6 (PubChem release 2019.06.18)

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3.1.2 InChI

InChI=1S/C12H22O11/c13-1-3-5(15)6(16)9(19)12(22-3)23-10-4(2-14)21-11(20)8(18)7(10)17/h3-20H,1-2H2/t3?,4?,5-,6?,7?,8?,9?,10-,11+,12-/m1/s1

Computed by InChI 1.0.5 (PubChem release 2019.06.18)

PubChem

3.1.3 InChIKey

GUBGYTABKSRVRQ-JTGJSBPZSA-N

Computed by InChI 1.0.5 (PubChem release 2019.06.18)

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3.1.4 Canonical SMILES

C(C1C(C(C(C(O1)OC2C(OC(C(C2O)O)O)CO)O)O)O)O

Computed by OEChem 2.1.5 (PubChem release 2019.06.18)

PubChem

3.1.5 Isomeric SMILES

C(C1[C@H](C(C([C@H](O1)O[C@@H]2C(O[C@@H](C(C2O)O)O)CO)O)O)O)O

Computed by OEChem 2.1.5 (PubChem release 2019.06.18)

PubChem

Case No.: IPR2023-00206
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3.2 Molecular Formula

C12H22O11

Computed by PubChem 2.1 (PubChem release 2019.06.18)

PubChem

3.3 Synonyms

3.3.1 Depositor-Supplied Synonyms

SCHEMBL12278702
Maltodextrin - dextrose equivalent 10-15

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4 Chemical and Physical Properties

4.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	342.30	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3-AA	-4.7	Computed by XLogP3 3.0 (PubChem release 2019.06.18)
Hydrogen Bond Donor Count	8	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Hydrogen Bond Acceptor Count	11	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Rotatable Bond Count	4	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Exact Mass	342.11621151	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	342.11621151	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	190 $Å^2$	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Heavy Atom Count	23	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	382	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	4	Computed by PubChem
Undefined Atom Stereocenter Count	6	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2019.01.04)

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5 Related Records

5.1 Related Compounds with Annotation

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5.2 Related Compounds

Same Connectivity	376 Records
Same Isotope	354 Records
Same Parent, Connectivity	749 Records
Same Parent, Isotope	720 Records
Same Parent, Exact	2 Records
Mixtures, Components, and Neutralized Forms	1 Record
Similar Compounds	8,402 Records

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5.3 Substances

5.3.1 Related Substances

All	4 Records
Same	3 Records
Mixture	1 Record

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5.3.2 Substances by Category

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6 Chemical Vendors

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7 Patents

7.1 Depositor-Supplied Patent Identifiers

- PubChem

Link to all deposited patent identifiers

- PubChem

8 Information Sources

FILTER BY SOURCE ALL SOURCES

1. PubChem
   https://pubchem.ncbi.nlm.nih.gov