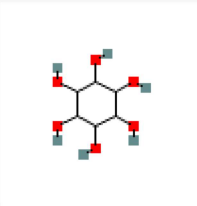

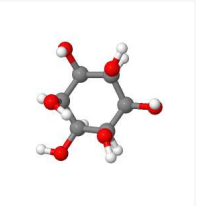



COMPOUND SUMMARY

Inositol

PubChem CID	892
Structure	 2D  3D  Crystal
Chemical Safety	 Irritant Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	C₆H₁₂O₆
Synonyms	inositol myo-inositol Scyllo-inositol epi-Inositol Muco-Inositol View More...
Molecular Weight	180.16 g/mol <i>Computed by PubChem 2.2 (PubChem release 2021.10.14)</i>
Dates	Create: 2004-09-16 Modify: 2024-07-20
Description	Myo-inositol is an inositol having myo- configuration. It has a role as a member of compatible osmolytes, a nutrient, an EC 3.1.4.11 (phosphoinositide phospholipase C) inhibitor, a human metabolite, a Daph

nia magna metabolite, a *Saccharomyces cerevisiae* metabolite, an *Escherichia coli* metabolite and a mouse metabolite.

▶ [ChEBI](#)

An isomer of [glucose](#) that has traditionally been considered to be a B vitamin although it has an uncertain status as a vitamin and a deficiency syndrome has not been identified in man. (From Martindale, The Extra Pharmacopoeia, 30th ed, p1379) Inositol phospholipids are important in signal transduction. Scyllitol has been investigated for the treatment of Alzheimer Disease.

▶ [DrugBank](#)

Inositol is a collection of nine different stereoisomers but the name is usually used to describe only the most common type of inositol, myo-inositol. Myo-inositol is the cis-1,2,3,5-trans-4,6-cyclohexanehexol and it is prepared from an aqueous extract of corn kernels by precipitation and hydrolysis of crude [phytate](#). These molecules have structural similarities to [glucose](#) and are involved in cellular signaling. It is considered a pseudovitamin as it is a molecule that does not qualify to be an essential vitamin because even though its presence is vital in the body, a deficiency in this molecule does not translate into disease conditions. Inositol can be found as an ingredient of OTC products by Health Canada but all current products whose main ingredient is inositol are discontinued. By the FDA, inositol is considered in the list of specific substances affirmed as generally recognized as safe (GRAS).

▶ [DrugBank](#)

[View More...](#)

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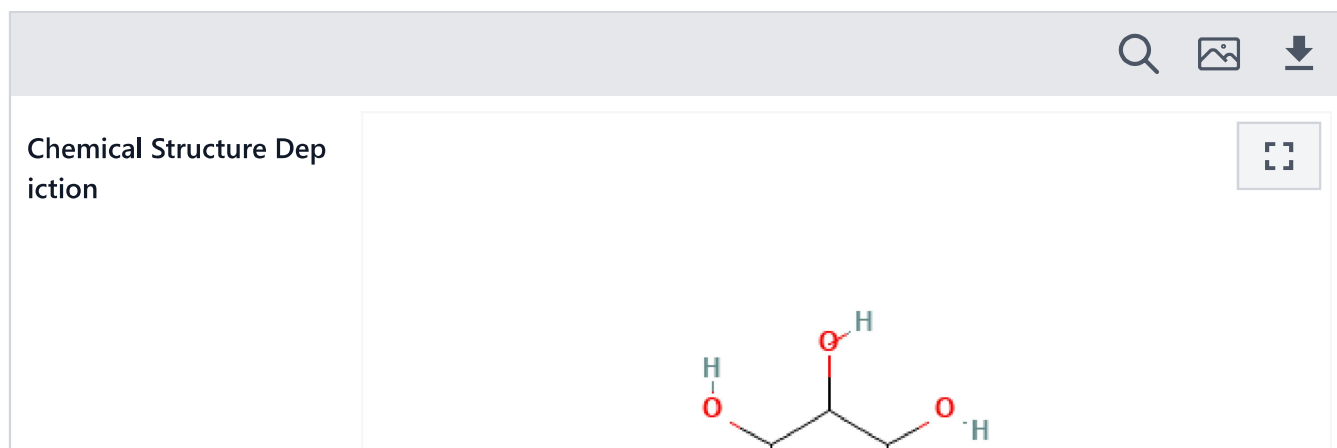
4 Spectral Information

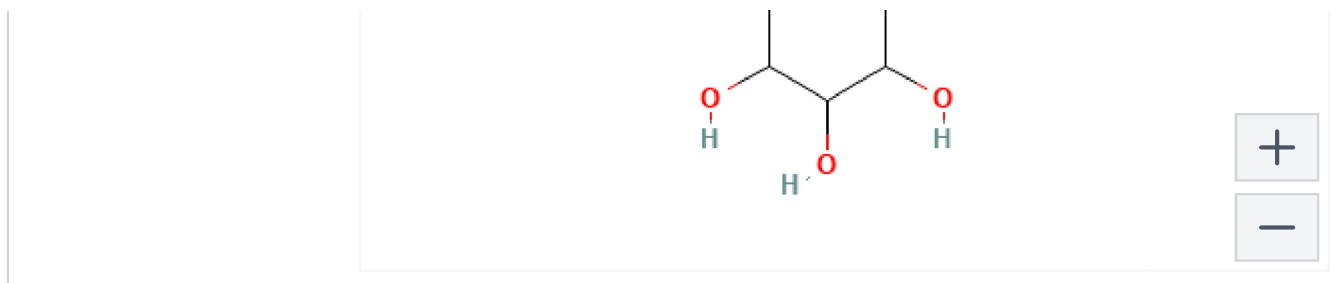
5 Related Records	∨
6 Chemical Vendors	
7 Drug and Medication Information	∨
8 Food Additives and Ingredients	∨
9 Pharmacology and Biochemistry	∨
10 Use and Manufacturing	∨
11 Safety and Hazards	∨
12 Toxicity	∨
13 Associated Disorders and Diseases	
14 Literature	∨
15 Patents	∨
16 Interactions and Pathways	∨
17 Biological Test Results	∨
18 Taxonomy	
19 Classification	∨
20 Information Sources	

1 Structures



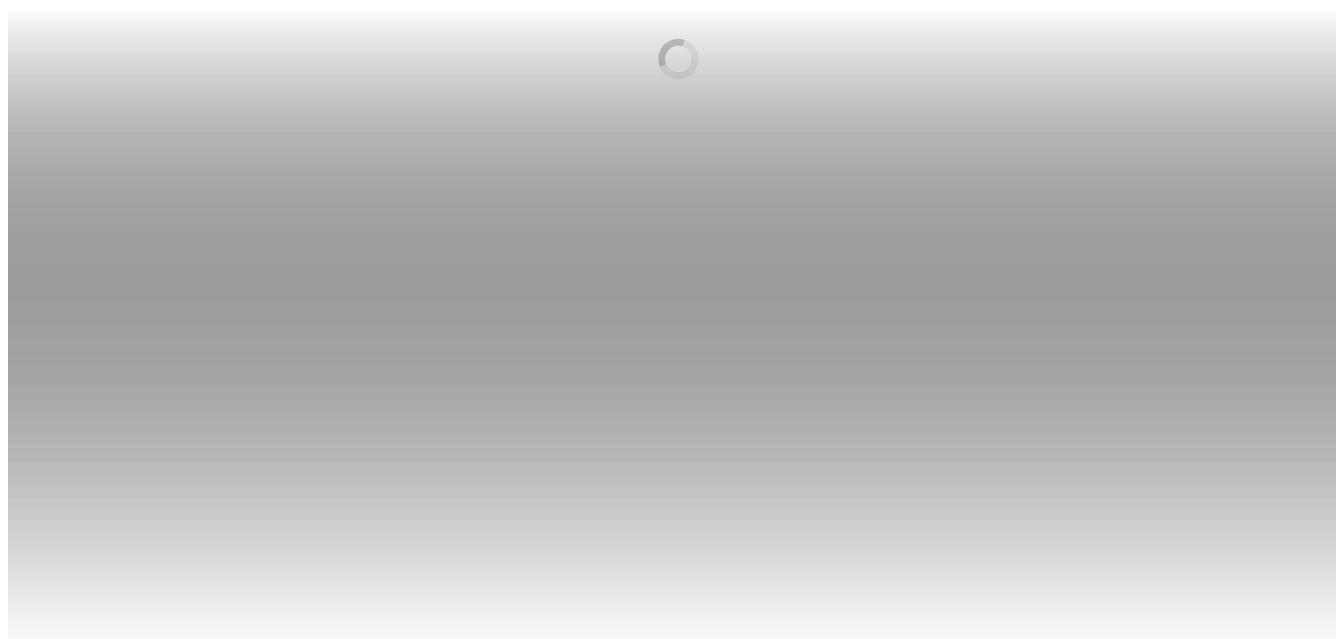
1.1 2D Structure





▶ PubChem

1.2 3D Conformer

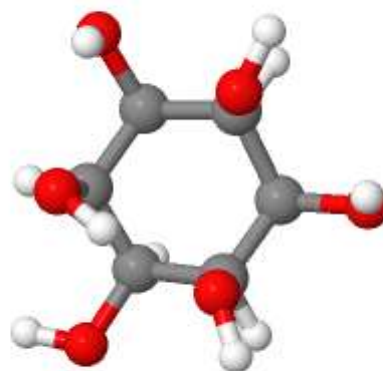


▶ PubChem

1.3 Crystal Structures



1 of 8	View All
COD Number	1543051
Associated Article	Bekö, Sándor L.; Alig, Edith; Schmidt, Martin U.; van de Streek, Jacco. On the correlation between hydrogen bonding and melting points in the inositols. IUCrJ 2013;1(1):61-73. DOI: 10.1107/s2052252513026511

Crystal Structure Depiction**Hermann-Mauguin space group symbol** P 2₁/n**Hall space group symbol** -P 2₁yn**Space group number** 14**a** 11.58792 Å**b** 12.2101 Å**c** 5.25364 Å**α** 90 °**β** 90.5649 °**γ** 90 °**Z** 4[▶ Crystallography Open Database \(COD\)](#)

2 Names and Identifiers



2.1 Computed Descriptors



2.1.1 IUPAC Name

