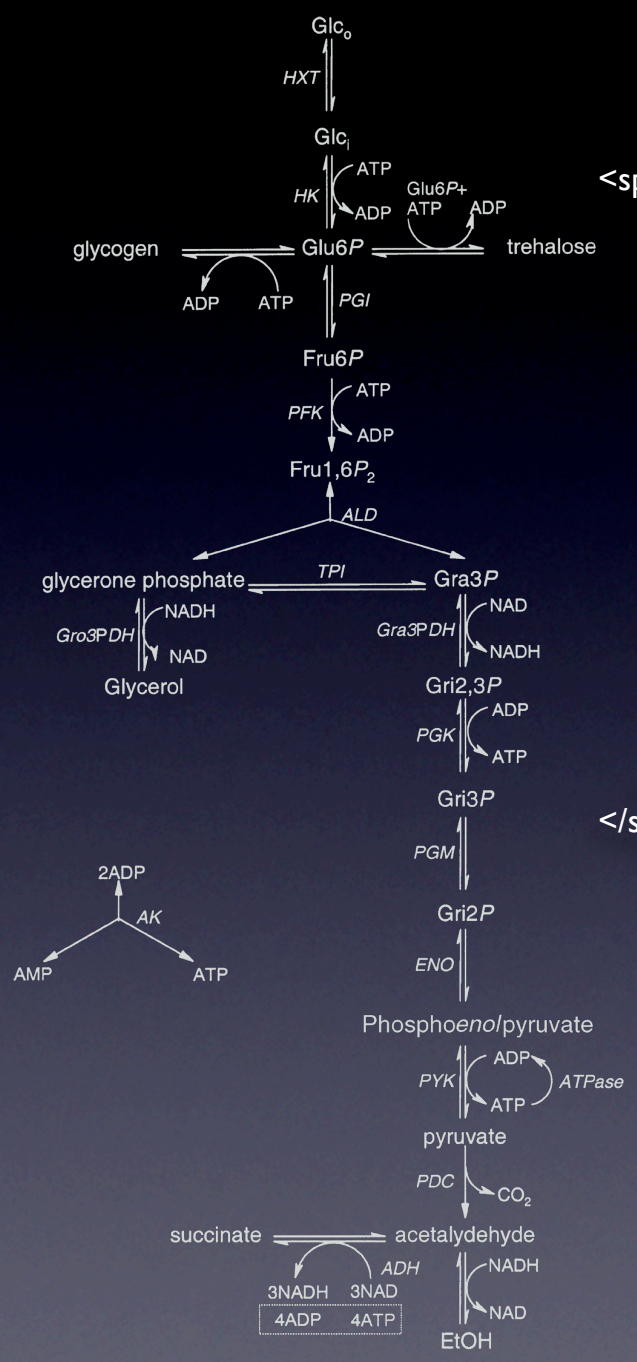


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        compartment="cytosol" initialConcentration="0.07">
      <annotation>
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                 xmlns:bqbiol="http://biomodels.net/biology-qualifiers/"
                 xmlns:bqmodel="http://biomodels.net/model-qualifiers/" >
          <rdf:Description rdf:about="#metaid_0000012">
              <bqbiol:is>
                <rdf:Bag>
                  <rdf:li rdf:resource="urn:miriam:chebi:26055"/>
                  <rdf:li rdf:resource="urn:miriam:kegg.compound:C00074"/>
                </rdf:Bag>
              </bqbiol:is>
          </rdf:Description>
        </rdf:RDF>
    </annotation>
</species>
```

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Chemical Entities of Biological Interest (ChEBI)

http://www.ebi.ac.uk/chebi/

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09 May 2008 - Chemical Structure Searching - Beta Version

Chemical structure searching is now available in ChEBI on the Advanced Search Page. It allows you to perform substructure, similarity and identity

ChEBI Home

ChEBI Search

Wildcard character is %

Example: "iron%", "InChI=1/H2O/h1H2"

ChEBI User Group Meeting! We are delighted to announce our first ChEBI User Group Meeting which will take place on the 19th and 20th May 2008. This is an opportunity to meet the ChEBI team, influence future developments and provide valuable feedback to the ChEBI project. Further information and registration details can be found on the ChEBI User Group Meeting page.

Page Contents

1. Introduction

Chemical **E**ntities of **B**iological Interest (**ChEBI**) is a freely available dictionary of molecular entities focused on 'small' chemical compounds. The term 'molecular entity' refers to any constitutionally or isotopically distinct atom, molecule, ion, ion pair, radical, radical ion, complex, conformer, etc., identifiable as a separately distinguishable entity. The molecular entities in question are either products of nature or synthetic products used to intervene in the processes of living organisms.

ChEBI encompasses an ontological classification, whereby the relationships between molecular entities or classes of entities and their parents and/or children are specified.

ChEBI uses nomenclature, symbolism and terminology endorsed by the following international scientific bodies:

- International Union of Pure and Applied Chemistry (IUPAC)
- Nomenclature Committee of the International Union of Biochemistry and Molecular Biology (NC-IUBMB)

Molecules directly encoded by the genome (e.g. nucleic acids, proteins and peptides derived from proteins by cleavage) are *not* as a rule included in ChEBI.

All data in the database is non-proprietary or is derived from a non-proprietary source. It is thus freely accessible and available to anyone. In addition, each data item is fully traceable and explicitly referenced to the original source.

Top

2. Entity of the month

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phosphoenolpyruvic acid (CHEBI:44897)

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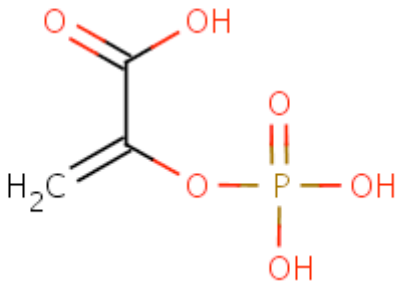
phosphoenolpyruvic acid (CHEBI:44897)

Main | Automatic Xrefs



ChEBI Name	phosphoenolpyruvic acid
ChEBI ID	CHEBI:44897
ChEBI ASCII Name	phosphoenolpyruvic acid
Last Modified	13 September 2007

☑ Image
☐ Applet

Molfile

InChI	InChI=1/C3H5O6P/c1-2(3(4)5)9-10(6,7)8/h1H2,(H,4,5)(H2,6,7,8)
SMILES	OC(=O)C(=C)OP(O)(O)=O

Formula	Source
C3H5O6P	KEGG COMPOUND

Charge	0
Mass	168.04196

ChEBI Ontology

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phosphoenolpyruvic acid (CHEBI:44897)

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Formula	Source
C3H5O6P	KEGG COMPOUND

Charge	0
Mass	168.04196

ChEBI Ontology

Tree view

Parents	phospho*enol*pyruvic acid (CHEBI:44897) **is conjugate acid of** phospho*enol*pyruvate (CHEBI:18021) phospho*enol*pyruvic acid (CHEBI:44897) **has functional parent** acrylic acid (CHEBI:18308) phospho*enol*pyruvic acid (CHEBI:44897) **is a** carboxyalkyl phosphates (CHEBI:36952)
Children	phospho*enol*pyruvate (CHEBI:18021) **is conjugate base of** phospho*enol*pyruvic acid (CHEBI:44897)

IUPAC Name

2-(phosphonooxy)prop-2-enoic acid

Synonyms	Sources
2-(phosphonooxy)-2-propenoic acid	ChemIDplus
2-PHOSPHOENOLPYRUVIC ACID	MSDchem
PEP	KEGG COMPOUND
PHOSPHOENOLPYRUVATE	MSDchem
Phosphoenolpyruvic acid	KEGG COMPOUND

Database Links	Databases
C00074	KEGG COMPOUND
PEP	MSDchem

Registry Numbers	Types	Sources
138-08-9	CAS Registry Number	KEGG COMPOUND
138-08-9	CAS Registry Number	ChemIDplus

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phosphoenolpyruvic acid (CHEBI:44897)

KEGG COMPOUND: C00074

http://www.genome.ad.jp/dbget-bin/www_bget?cpd:C00074

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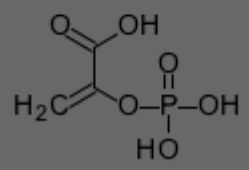
KEGG **COMPOUND: C00074**

Help

Entry	C00074 Compound
Name	Phosphoenolpyruvate; Phosphoenolpyruvic acid; PEP
Formula	C3H5O6P
Mass	167.9824
Structure	 C00074 Mol file KCF file DB search Jmol KegDraw
Reaction	R00199 R00200 R00206 R00208 R00341 R00345 R00346 R00430 R00431 R00572 R00658 R00659 R00660 R00661 R00724 R00726 R01012 R01138 R01804 R01826 R01858 R02320 R02628 R02769 R03254 R03460 R04435 R06591 R07476
Pathway	PATH: map00010 Glycolysis / Gluconeogenesis PATH: map00020 Citrate cycle (TCA cycle) PATH: map00400 Phenylalanine, tyrosine and tryptophan biosynthesis PATH: map00440 Aminophosphonate metabolism PATH: map00620 Pyruvate metabolism PATH: map00710 Carbon fixation PATH: map00720 Reductive carboxylate cycle (CO2 fixation) PATH: map02060 Phosphotransferase system (PTS)
Enzyme	2.5.1.7 2.5.1.19 2.5.1.54 2.5.1.55 2.5.1.56 2.5.1.57 2.7.1.11 (E) 2.7.1.40 2.7.1.121 2.7.3.9 2.7.9.1 2.7.9.2 3.1.3.60 4.1.1.31 4.1.1.32 4.1.1.38 4.1.1.49 4.2.1.11 4.4.1.19 5.4.2.9
Other DBs	CAS: 138-08-9 PubChem: 3374 ChEBI: 18021 44897 PDB-CCD: PEP 3DMET: B00019

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phosphoenolpyruvate (CHEBI:18021)

http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:18021

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phosphoenolpyruvate (CHEBI:18021)

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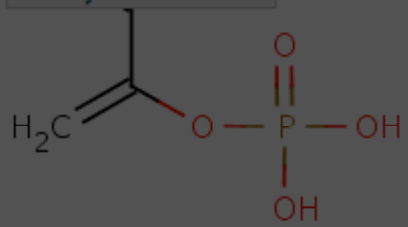
Similarity Search
Identity Search



ChEBI Name	phosphoenolpyruvate
ChEBI ID	CHEBI:18021
ChEBI ASCII Name	phosphoenolpyruvate
Last Modified	07 November 2006

☑ Image
☐ Applet

Molfile

InChI	InChI=1/C3H5O6P/c1-2(3(4)5)9-10(6,7)8/h1H2,(H,4,5)(H2,6,7,8)/p-1
SMILES	OP(O)(=O)OC(=C)C([O-])=O

Formula	Source
C3H4O6P	ChemIDplus

Charge	-1
Mass	167.03402

ChEBI Ontology

PDB-CCD: PEP
3DMET: B00019

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phosphoenolpyruvate (CHEBI:18021)

phosphoenolpyruvate – PubChem Public Chemical Database

http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?sid=3374

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PubChem » Substance Summary

ASN.1 XML SDF

phosphoenolpyruvate - Substance Summary

(SID: 3374)

Table of Contents

Drug and Chemical Info: (Total:1)

Phosphoenolpyruvate

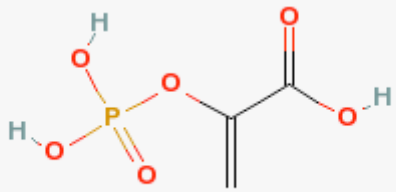
Classification

Organic Chemicals
Carboxylic Acids
Hydroxy Acids
Phosphoenolpyruvate

PubMed via MeSH Choose by Subheadings:

administration and dosage	analogs and derivatives	analysis
antagonists and inhibitors	biosynthesis	blood
chemical synthesis	chemistry	diagnostic use
immunology	isolation and purification	metabolism
pharmacokinetics	pharmacology	physiology

Compound Displayed PubChem



Compound ID	**1005**	
Molecular Weight	168.041961 [g/mol]	
Molecular Formula	$C_3H_5O_6P$	
XLogP	-1.3	
H-Bond Donor	3	
H-Bond Acceptor	6	

Links

Chemical Structure Search

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phosphoenolpyruvate (CHEBI:18021)

phosphoenolpyruvate – PubChem Public Chemical Database

http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?sid=3374

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Rotatable Bond Count	3
Exact Mass	167.982374
MonoIsotopic Mass	167.982374
Topological Polar Surface Area	104
Heavy Atom Count	10
Formal Charge	0
Complexity	201
Isotope Atom Count	0
Defined Atom StereoCenter Count	0
Undefined Atom StereoCenter Count	0
Defined Bond StereoCenter Count	0
Undefined Bond StereoCenter Count	0
Covalently-Bonded Unit Count	1

Descriptors Computed from Structure:

IUPAC Name: 2-phosphonooxyprop-2-enoic acid
Canonical SMILES: C=C(C(=O)O)OP(=O)(O)O
InChI: InChI=1/C3H5O6P/c1-2(3(4)5)9-10(6,7)8/h1H2,(H,4,5)(H2,6,7,8)/f/h4,6-7H

Substance Info:

SID: 3374
Deposit Date: 2005-06-24
Modify Date: 2008-04-02

CID: 1005
Create Date: 2004-09-16

Related Substances:
Same: 55 Links
Same, Connectivity: 58 Links

Similar Substances: 119 Links

InChI From ChEBI for Phosphoenolpyruvate

InChI=1/C3H5O6P/c1-2(3(4)5)9-10(6,7)8/h1H2,(H,4,5)(H2,6,7,8)/f/h4,6-7H

InChI From PubChem for Phosphoenolpyruvate

InChI=1/C3H5O6P/c1-2(3(4)5)9-10(6,7)8/h1H2,(H,4,5)(H2,6,7,8)/p-1