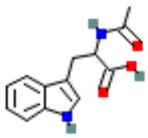
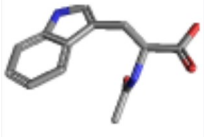
COMPOUND SUMMARY

N-Acetyl-DL-tryptophan

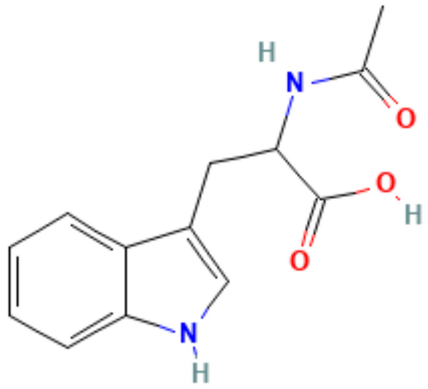
PubChem CID	2002
Structure	 2D  3D
Chemical Safety	Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_{13}H_{14}N_2O_3$
Synonyms	N-Acetyl-DL-tryptophan 87-32-1 Ac-DL-Trp-OH N-Acetyltryptophan DL-Acetyltryptophan View More...
Molecular Weight	246.26 g/mol *Computed by PubChem 2.2 (PubChem release 2021.10.14)*
Dates	Create: 2005-03-25 Modify: 2024-01-06
Description	N-acetyltryptophan is an N-acetylamino acid that is the N-acetyl derivative of tryptophan. It has a role as a metabolite. It is a N-acetyl-amino acid and a tryptophan derivative. It is a conjugate acid of a N-acetyltryptophanate. ▸ ChEBI N-Acetyl-DL-tryptophan is a natural product found in Aspergillus nidulans, Penicillium commune, and other organisms with data available. ▸ LOTUS - the natural products occurrence database

1 Structures

1.1 2D Structure

Structure Search | Get Image | Download Coordinates

Chemical Structure Depiction



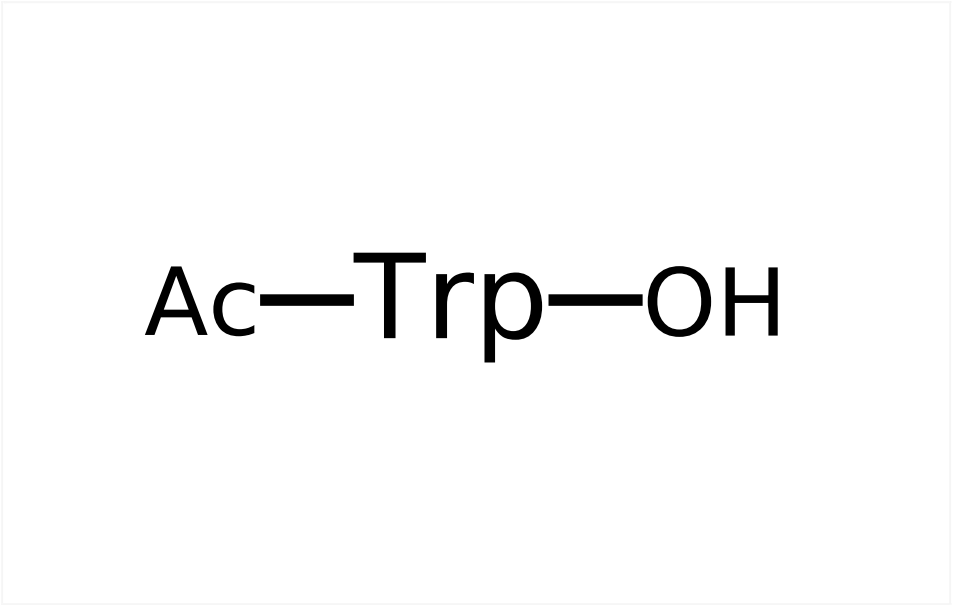
PubChem

1.2 3D Conformer

UPDATING...

PubChem

2 Biologic Description

SVG Image	
IUPAC Condensed	Ac-DL-Trp-OH
Sequence	W
PLN	[acetyl]-W-OH
HELM	PEPTIDE1{[ac].(W,[dW])}$$$$V2.0
IUPAC	N-acetyl-DL-tryptophan

PubChem

3 Names and Identifiers

3.1 Computed Descriptors

3.1.1 IUPAC Name

2-acetamido-3-(1*H*-indol-3-yl)propanoic acid

Computed by Lexichem TK 2.7.0 (PubChem release 2021.10.14)

PubChem

3.1.2 InChI

InChI=1S/C13H14N2O3/c1-8(16)15-12(13(17)18)6-9-7-14-11-5-3-2-4-10(9)11/h2-5,7,12,14H,6H2,1H3,(H,15,16)(H,17,18)

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

PubChem

3.1.3 InChIKey

DZTHIGRZJZPRDV-UHFFFAOYSA-N

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

- PubChem

3.1.4 Canonical SMILES

CC(=O)NC(CC1=CNC2=CC=CC=C21)C(=O)O

Computed by OEChem 2.3.0 (PubChem release 2021.10.14)

- PubChem

3.2 Molecular Formula

$C_{13}H_{14}N_2O_3$

Computed by PubChem 2.2 (PubChem release 2021.10.14)

- PubChem

3.3 Other Identifiers

3.3.1 CAS

87-32-1

- CAS Common Chemistry; ChemIDplus; DTP/NCI; EPA Chemicals under the TSCA; EPA DSSTox; Euro...

1218-34-4

- DTP/NCI

3.3.2 Deprecated CAS

10385-85-0

- ChemIDplus

3.3.3 European Community (EC) Number

201-739-3

- European Chemicals Agency (ECHA)

3.3.4 UNII

4460NBV53F

- FDA Global Substance Registration System (GSRS)

3.3.5 ChEMBL ID

CHEMBL1905494

- ChEMBL

3.3.6 DSSTox Substance ID

DTXSID40861672

- EPA DSSTox

3.3.7 Metabolomics Workbench ID

103793

- Metabolomics Workbench

3.3.8 NCI Thesaurus Code

C77305

- NCI Thesaurus (NCIt)

3.3.9 NSC Number

90726

- DTP/NCI

49124

- DTP/NCI