Compound Summary for CID 92258

Phenylacetylglutamine

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PubChem CID:	92258
Chemical Names:	Phenylacetylglutamine; 28047-15-6; (S)-5-Amino-5-oxo-2-(2-phenylacetamido)pentanoic acid; Phenylacetyl-L-glutamine; Phenylacetyl L-Glutamine; PHENYLAC-GLN-OH More...
Molecular Formula:	$C_{13}H_{16}N_2O_4$
Molecular Weight:	264.281 g/mol
InChI Key:	JFLIEFSWGNOPJJ-JTQLQIEISA-N
Substance Registry:	FDA UNII

Phenylacetylglutamine is a product formed from the conjugation of phenylacetate and glutamine. Technically, it is the amino acid acetylation product of phenylacetate (or phenylbutyrate after beta-oxidation). Phenylacetylglutamine is a normal constituent of human urine, but other mammals such as the dog, cat, rat, monkey, sheep, and horse do not excrete this compound. Phenylacetyl-CoA and L-glutamine react to form phenylacetylglutamine and coenzyme A. The enzyme (glutamine N-acetyl transferase) that catalyzes this reaction has been purified from human liver mitochondria and shown to be a polypeptide species distinct from glycine-N-acyltransferase. Phenylacetylglutamine is a major nitrogenous metabolite that accumulates in uremia (PMID: 2791363, 8972626). It has been shown that over 50% of urine phenylacetylglutamine may be derived from kidney conjugation of free plasma phenylacetic acid and/or from the kidney's preferential filtration of conjugated phenylacetic acid (PMID: 6420430).

Metabolite Description from Human Metabolome Database (HMDB)

Contents

1 2D Structure

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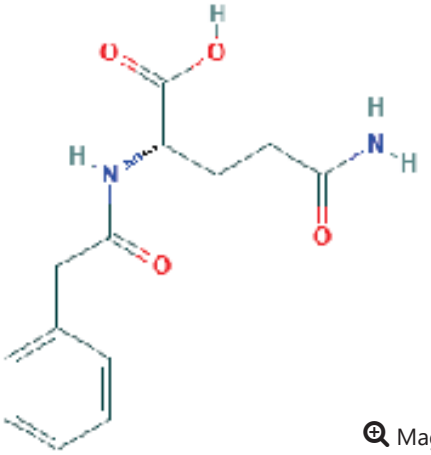

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2 3D Conformer

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3 Names and Identifiers

3.1 Computed Descriptors

3.1.1 IUPAC Name

(2S)-5-amino-5-oxo-2-[(2-phenylacetyl)amino]pentanoic acid

from PubChem

3.1.2 InChI

InChI=1S/C13H16N2O4/c14-11(16)7-6-10(13(18)19)15-12(17)8-9-4-2-1-3-5-9/h1-5,10H,6-8H2,(H2,14,16)(H,15,17)(H,18,19)/t10-/m0/s1

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3.1.3 InChI Key

JFLIEFSWGNOPJJ-JTQLQIEISA-N

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3.1.4 Canonical SMILES

C1=CC=C(C=C1)CC(=O)NC(CCC(=O)N)C(=O)O

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3.1.5 Isomeric SMILES

C1=CC=C(C=C1)CC(=O)N[C@@H](CCC(=O)N)C(=O)O

from PubChem

3.2 Molecular Formula

$C_{13}H_{16}N_2O_4$

from PubChem

3.3 Other Identifiers

3.3.1 CAS

28047-15-6

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