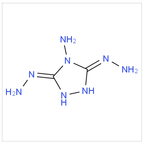

3D | Mol | Similar

4H-1,2,4-Triazol-4-amine,3,5-dihydrazinyl-

Iupac Name: 3,5-dihydrazinyl-1,2,4-triazol-4-amine

CAS No.: 1614-08-0

Molecular Weight: 144.142

Modify Date.: 2022-11-07 21:00

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Directory

1. Names and Identifiers
2. Properties
3.Synthesis Route
4.Precursor and Product
5.Computational chemical data

1. Names and Identifiers

1.1 Name

4H-1,2,4-Triazol-4-amine,3,5-dihydrazinyl-

1.2 Synonyms

1,2,4-Triazolidine-3,5-dione,4-amino-, dihydrazone (9CI)

3,5-Dihydrazino-4H-1,2,4-triazol-4-amine

3,5-dihydrazinyl-1,2,4-triazol-4-amine

4-Amino-3,5-dihydrazino-1,2,4(4H)-triazole

4-Amino-3,5-dihydrazino-4H-1,2,4-triazole

4-Aminodihydrazino-1,2,4-triazole

4H-1,2,4-Triazol-4-amine, 3,5-bis(hydrazinyl)-

4H-1,2,4-Triazole, 4-amino-3,5-dihydrazino-(7CI,8CI)

View all

1.3 CAS No.

1614-08-0

1.4 CID

350583

1.5 Molecular Formula

C2H8N8 (isomer)

1.6 Inchi

InChI=1S/C2H8N8/c3-6-1-8-9-2(7-4)10(1)5/h3-5H2,(H,6,8)(H,7,9)

1.7 InChIkey

FQYGPCLWFSTWSD-UHFFFAOYSA-N

1.8 Canonical Smiles

C1(=NN=C(N1N)NN)NN

1.9 Isomers Smiles

C1(=NN=C(N1N)NN)NN

2. Properties

2.1 Density

2.57

2.1 Boiling point

494.4°Cat760mmHg

2.1 Refractive index

2.178

2.1 Flash Point

252.8°C

2.1 PSA

139.29000

2.1 logP

-2.26 (Predicted)

3. Synthesis Route

1614-08-0 Total: 4 Synthesis Route

124-46-9

1 Suppliers

1614-08-0

Literatures:
Leonova, T. G.; Larionov, S. V.; Sheludyakova, L. A. J. Gen. Chem. USSR (Eng l. Transl.), 1987 , vol. 57, # 11 p. 2590 - 2594,2307 - 2310

Yield: null

Picture loading...

593-85-1

224 Suppliers

Picture loading...

1614-08-0

Literatures:
Stolle; Bowles Chemische Berichte, 1908 , vol. 41, p. 1101

Yield: null

Picture loading...

127099-85-8

Picture loading...

1614-08-0

Literatures:
Stolle; Krauch Journal fuer Praktische Chemie (Leipzig), 1913 , vol. <2>88, p. 312

Yield: null

View all

4. Precursor and Product

precursor:

Picture loading... 593-85-1

Picture loading... 124-46-9

Picture loading... 127099-85-8

5. Computational chemical data

Molecular Weight: 144.142g/mol

Molecular Formula: $C_2H_8N_8$

Compound Is Canonicalized: True

XLogP3-AA: -1.1

Exact Mass: 144.08719229

Monoisotopic Mass: 144.08719229

Complexity: 91.4

Rotatable Bond Count: 2

Hydrogen Bond Donor Count: 5

Hydrogen Bond Acceptor Count: 7

Topological Polar Surface Area: 133

Heavy Atom Count: 10

Defined Atom Stereocenter Count: 0

Undefined Atom Stereocenter Count: 0

Defined Bond Stereocenter Count: 0

Undefined Bond Stereocenter Count: 0

Isotope Atom Count: 0

Covalently-Bonded Unit Count: 1

CACTVS Substructure Key Fingerprint: AAADccBDwAAAAAAAAAAAAAAAAAAAAAWAAAAAAAAAAAAAAAAAABgAAABAAYAAAAAAAAAAABEAZqEAAiAAAAJAAQAAsAAIIFIAAAAACACAAAAAAAAAAQAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA==

7. Realated Product Infomation

350707-64-1
4,6-Dihydrazinyl-N-(2-

16974-50-8
Pyrimidine,2,4-dihydrazinyl-

61-82-5
Triazol-3-amine

65312-61-0
(4H)-1,2,4-triazol-3-amine

1782530-21-5
2-(Methoxymethyl)triaz

194469-74-4
2H-1,2,3-Triazol-4-amine hydrochloride

4922-98-9
5-PHENYL-1H-1,2,4-TRIAZOL-3-

Recently Updated : 2228040-39-7 | 1154936-36-3 | 1484160-26-0 | 1822564-98-6 | 1824322-92-0 | 1368497-71-5 | 643039-73-0 | 1823974-25-9 | 885901-09-7 | 1781028-63-4