



1,3,5-Trimethyl-2,4,6-trinitrobenzene

Iupac Name: 1,3,5-trimethyl-2,4,6-trinitrobenzene
 CAS No.: **602-96-0**
 Molecular Weight: 255.186
 Modify Date.: 2022-11-25 21:24
 Introduction: Nitro derivatives of toluene. Explosive. 1,3,5-Trimethyl-2,4,6-trinitrobenzeneSupplier

[Request For Quotation](#)

3D Mol Similar

1. Names and Identifiers

1.1 Name

1,3,5-Trimethyl-2,4,6-trinitrobenzene

1.2 Synonyms

2,4,6-TrinitroMesitylene Benzene, 1,3,5-trimethyl-2,4,6-trinitro-
 Mesitylene, 2,4,6-trinitro- NSC 29088
 Trinitromesitylene

1.3 CAS No.

602-96-0

1.4 CID

11771

1.5 Molecular Formula

C₉H₉N₃O₆ (isomer)

1.6 Inchi

InChI=1S/C9H9N3O6/c1-4-7(10(13)14)5(2)9(12(17)18)6(3)8(4)11(15)16/h1-3H3

1.7 InChIkey

YVJXCMCIFUNDO-UHFFFAOYSA-N

1.8 Canonical Smiles

CC1=C(C(=C(C(=C1[N+](=O)[O-])C)[N+](=O)[O-])C)[N+](=O)[O-]

1.9 Isomers Smiles

CC1=C(C(=C(C(=C1[N+](=O)[O-])C)[N+](=O)[O-])C)[N+](=O)[O-]

Directory

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2. Properties

2.1 Density

1.468

2.1 Melting point

238.2°C

2.1 Boiling point

366.1°C at 760 mmHg

2.1 Refractive index

1.611

2.1 Flash Point

173.4°C

2.1 PSA

137.46000

2.1 logP

3.90600

2.1 Chemical Properties

White Powder

3. Use and Manufacturing

3.1 Usage

Nitro derivatives of toluene. Explosive. 1,3,5-Trimethyl-2,4,6-trinitrobenzeneSupplier

4. Safety and Handling

4.1 Safety Statements

An unstable substance forbidden from transport. When heated to decomposition it emits toxic vapors of Cl⁻.

4.1 Safety

An unstable substance forbidden from transport. When heated to decomposition it emits toxic vapors of Cl⁻.

5. MSDS

2.Hazard identification

2.1 Classification of the substance or mixture

no data available

2.2 GHS label elements, including precautionary statements

Pictogram(s)	no data available
Signal word	no data available
Hazard statement(s)	no data available
Precaution statement(s)	
Prevention	no data available

[View all](#)

6. Synthesis Route

602-96-0 Total: 2 Synthesis Route

Literatures:
 Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), , # 14 p. 1591 - 1598
Yield: null

Literatures:
 Kunckell; Hildebrandt Chemische Berichte, 1901 , vol. 34, p. 1827
Yield: null

7. Precursor and Product

precursor:

108-67-8

156641-43-9

product :

3102-70-3

4463-03-0

4380-92-1

8. Other Information

8.0 Chemical Properties

White Powder

8.1 Uses

Nitro derivatives of toluene. Explosive.

9. Computational chemical data

Molecular Weight: 255.186g/mol
 Molecular Formula: C₉H₉N₃O₆
 Compound Is Canonicalized: True
 XLogP3-AA: 2.5
 Exact Mass: 255.04913502
 Monoisotopic Mass: 255.04913502
 Complexity: 295
 Rotatable Bond Count: 0
 Hydrogen Bond Donor Count: 0
 Hydrogen Bond Acceptor Count: 6
 Topological Polar Surface Area: 138
 Heavy Atom Count: 18
 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: AAADccBzOAABAAAAHAAEAAAAAIBGAACwIA
 QQACBAGRAQwCCAAAGAAAgIAAARIlOICKAONGAIBggAAlYAcQgEAOCAACAAQCAAAQAAQACAAQAAAAAAAAAAAAAAAA==

10. Recommended Suppliers

Global 3 Suppliers [View all >>](#)

Hangzhou Keyingchem Co.,Ltd Tel:+86-571-85378921	1,3,5-Trimethyl-2,4,6-trinitrobenzene Purity:99% Packing: 200kg/bag FOB Price: Time: 2019/05/06	Inquire
Livchem Logistics GmbH Tel:+49 (0) 69 3800 2685	1,3,5-Trimethyl-2,4,6-trinitrobenzene Purity:99% Packing: 200kg/bag FOB Price: Time: 2019/02/25	Inquire
SelectLab Chemicals GmbH Tel:+49-2383-919350	1,3,5-Trimethyl-2,4,6-trinitrobenzene;Trinitromesitylene Purity:99% Packing: 200kg/bag FOB Price: Time: 2022/01/01	Inquire

11. Related Product Infomation

602-23-3	132699-65-1	1630-09-7	3058-38-6	364-44-3	125010-19-7	35074-90-9
1,2,4-Trimethyl-3,5,6-trinitrobenzene	1-N,3-N,5-N-trimethyl-2,4,6-trinitrobenzene	1,3-DICHLORO-2,4,6-trinitrobenzene	2,4,6-trinitrobenzene-1,3,5-triamine	1-fluoro-2,4,6-trinitrobenzene	1,3,5-Tripieryl-2,4,6-trinitrobenzene	2-Ethenyl-1,3,5-trinitrobenzene

Recently Updated : 136890-19-2 424818-58-6 68628-69-3 425372-20-9 482638-18-6 897544-01-3 488785-96-2 496965-16-3 583030-31-3
 1937282-88-6