

## **Specification Sheet**

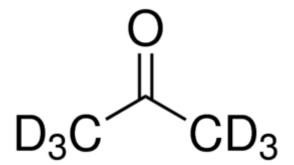
540331 Sigma-Aldrich

## Acetone-d.

99.9 atom % D

Synonym: Hexadeuteroacetone

- CAS Number <u>666-52-4</u>
- Linear Formula CD<sub>3</sub>COCD<sub>3</sub>
- Molecular Weight 64.12
- Beilstein/REAXYS Number 1702935
- EC Number <u>211-563-9</u>
- MDL number <u>MFCD00044635</u>
- PubChem Substance ID 24878459<sup>№</sup>



| SKU-Pack Size | Availability                           | Pack Size | Price<br>(SGD) | Quantity |
|---------------|--|-----------|----------------|----------|
| 540331-10ML   | Estimated to ship on 04.05.2021 - FROM | 10 mL     |                | 0        |

## **Properties**

| Related Categories | Acetone, Acetone-d <sub>6</sub> , NMR Solvents, Solvent by Type, Solvent by Application, |
|--------------------|--|
| vapor density      | 2 (vs air)   |
| vapor pressure     | 14.39 psi ( 55 °C)   |
|                    | 184 mmHg ( 20 °C)  |



## Sigma-Aldrich.

| 3.67 | psi ( | 20  | °C) |
|------|-------|-----|-----|
|      | P 1   | · · | -,  |

| isotopic purity  | 99.9 atom % D                           |
|------------------|---|
| assay            | 99% (CP)                                |
| form             | liquid                                  |
| expl. lim.       | 13.2 %                                  |
| impurities       | ≤0.0500% water water                    |
| refractive index | n20/D 1.355 (lit.)                      |
| bp               | 55.5 °C (lit.)                          |
| mp               | −93.8 °C (lit.)                         |
| density          | 0.872 g/mL at 25 °C (lit.)              |
| mass shift       | M+6                                     |
| storage temp.    | room temp                               |
| SMILES string    | [2H]C([2H])([2H])C(=O)C([2H])([2H])[2H] |
| InChI            | 1S/C3H6O/c1-3(2)4/h1-2H3/i1D3,2D3       |
| InChI key        | CSCPPACGZOOCGX-WFGJKAKNSA-N             |
|                  |   |

