

Specification Sheet

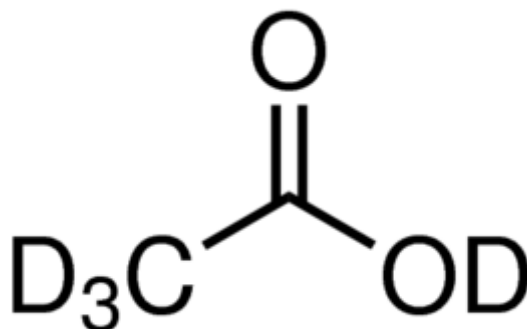
151785 Sigma-Aldrich

Acetic acid-d₄

≥99.5 atom % D

Synonym: **Acetic-d₃ acid-d**, Tetradeuteroacetic acid

- CAS Number [1186-52-3](#)
- Linear Formula CD₃CO₂D
- Molecular Weight 64.08
- Beilstein/REAXYS Number 1748971
- EC Number [214-693-4](#)
- MDL number [MFCD00051051](#)
- PubChem Substance ID [24848852](#)
- NACRES NA.21



Properties

Related Categories	A , Acetic acid-d₄ , Acids , Acids & Bases , Alphabetical Listings ,
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Quality Level	100
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vapor density	2.07 (vs air)
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vapor pressure	11.4 mmHg (20 °C)
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isotopic purity	≥99.5 atom % D
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assay	≥99% (CP)
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form	liquid
autoignition temp.	800 °F
expl. lim.	16 %
application(s)	NMR: suitable bio NMR: suitable
impurities	≤0.0500% water water
refractive index	$n_{20/D}$ 1.368 (lit.)
bp	115.5 °C (lit.)
mp	15-16 °C (lit.)
density	1.119 g/mL at 25 °C (lit.)
mass shift	M+4
storage temp.	room temp
SMILES string	<chem>[2H]OC(=O)C([2H])([2H])[2H]</chem>
InChI	1S/C2H4O2/c1-2(3)4/h1H3,(H,3,4)/i1D3/hD
InChI key	QTBSBXVTEAMEQO-GUEYOVJQSA-N



Description

General description

Acetic acid-d₄ (Tetradeuteroacetic acid), a deuterated carboxylic acid,^[1] is the tetradeuterated form of acetic acid. Its dissociation constant has been evaluated in deuterium oxide (D₂O) by an emf method.^[2]

Application

Acetic acid-d₄ has been used as a deuterated solvent for the dissolution of internal standard in qNMR (Quantitative Nuclear Magnetic Resonance) quantification experiments.^[2]

Acetic acid-d₄ may also be used as a deuterated solvent in the ¹H NMR spectral studies of the following:

- CB2, a CNBr peptide^[3]
- α - tocopherol succinate hydrophobically modified chitosan(CS-TOS)^[4]

Packaging

10x0.5, 10x1 mL in ampule
5, 10, 25, 50 g in glass bottle

