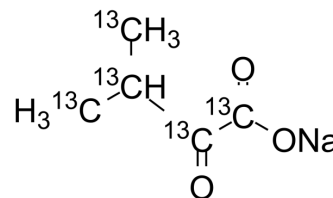


Sodium 3-methyl-2-oxobutanoate-¹³C₅

Cat. No.:	HY-W006057AS16		
CAS No.:	1173018-24-0		
Molecular Formula:	¹³ C ₅ H ₇ NaO ₃		
Molecular Weight:	143.06		
Target:	Endogenous Metabolite		
Pathway:	Metabolic Enzyme/Protease		
Storage:	Powder	-20°C	3 years
		4°C	2 years
	In solvent	-80°C	6 months
		-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

H₂O : ≥ 100 mg/mL (699.01 mM)
 * "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Solvent		1 mg	5 mg	10 mg
	Concentration	Mass			
1 mM			6.9901 mL	34.9504 mL	69.9007 mL
5 mM			1.3980 mL	6.9901 mL	13.9801 mL
10 mM			0.6990 mL	3.4950 mL	6.9901 mL

Please refer to the solubility information to select the appropriate solvent.

BIOLOGICAL ACTIVITY

Description

Sodium 3-methyl-2-oxobutanoate-¹³C₅ is the ¹³C labeled Sodium 3-methyl-2-oxobutanoate[1]. Sodium 3-methyl-2-oxobutanoate is a precursor of pantothenic acid in Escherichia coli[2][3][4].

In Vitro

Stable heavy isotopes of hydrogen, carbon, and other elements have been incorporated into drug molecules, largely as tracers for quantitation during the drug development process. Deuteration has gained attention because of its potential to affect the pharmacokinetic and metabolic profiles of drugs^[1].
 MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

- [1]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. *Ann Pharmacother*. 2019 Feb;53(2):211-216.
 [2]. MAAS WK, et al. alpha-Ketoisovaleric acid, a precursor of pantothenic acid in Escherichia coli. *J Bacteriol*. 1953 Apr;65(4):388-93.

[3]. Schauder P, et al. Oral administration of alpha-ketoisovaleric acid or valine in humans: blood kinetics and biochemical effects. J Lab Clin Med. 1984 Apr;103(4):597-605.

[4]. Coitinho AS, et al. Pharmacological evidence that alpha-ketoisovaleric acid induces convulsions through GABAergic and glutamatergic mechanisms in rats. Brain Res. 2001 Mar;989(1):68-73.

Caution: Product has not been fully validated for medical applications. For research use only.

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