Product Data Sheet

Monooctyl phthalate-d₄

 Cat. No.:
 HY-133671S

 CAS No.:
 1398065-74-1

 Molecular Formula:
 $C_{16}H_{18}D_4O_4$

Molecular Weight: 282.37

Target: Isotope-Labeled Compounds

Pathway: Others

Storage: Please store the product under the recommended conditions in the Certificate of

Analysis.

BIOLOGICAL ACTIVITY

Description	Monooctyl phthalate- d_4 (Mono-n-octyl phthalate- d_4) is a deuterium labeled Monooctyl phthalate (HY-133671). Monooctyl phthalate (Mono-n-octyl phthalate) exhibits antimycobacterial activity with a MIC of 20 μ g/mL ^{[1][2]} .
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]. Muniyan Rajiniraja, et al.In vitro inhibition potential of mono-n-octyl phthalate on Mycobacterium tuberculosis H37Ra: Possibility of binding to mycobacterial PknB-An in silico approach. Biotechnol Appl Biochem. 2018 Nov;65(6):865-875.

 $[2]. Russak \, EM, et \, al. \, Impact \, of \, Deuterium \, Substitution \, on \, the \, Pharmacokinetics \, of \, Pharmaceuticals. \, Ann \, Pharmacother. \, 2019 \, Feb; \\ 53(2): 211-246.$

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

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