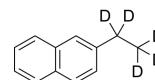


Product Datasheet

Physicochemical Properties	
Product Name	2-Ethynaphthalene-d5
Cat No.	V63667
Molecular Formula	C ₁₂ H ₇ D ₅
Molecular Weight	161.25
Exact Mass	161.125
CAS #	1219805-14-7
Appearance	Typically exists as solid at room temperature
Density	1.0±0.1 g/cm ³
Boiling Point	257.8±3.0 °C at 760 mmHg
Flash Point	104.4±0.0 °C
Vapour Pressure	0.0±0.2 mmHg at 25°C
Index of Refraction	1.602
LogP	4.44
tPSA	0
Hydrogen Bond Donor Count	0
Hydrogen Bond Acceptor Count	0
Rotatable Bond Count	1
Heavy Atom Count	12
Complexity	139
Defined Atom Stereocenter Count	0
SMILES	<chem>C([H])([H])(C1C=CC2C=CC=CC=2C=1)C([H])([H])[H]</chem>
InChi Key	RJTJVYSTUQWNI-ZBJDZAJPSA-N
InChi Code	InChI=1S/C12H12/c1-2-10-7-8-11-5-3-4-6-12(11)9-10/h3-9H,2H2,1H3/i1D3,2D2
Chemical Name	2-(1,1,2,2,2-pentadeuterioethyl)naphthalene
HS Tariff Code	2934.99.9001
Storage	Powder -20°C 3 years 4°C 2 years In solvent -80°C 6 months -20°C 1 month
Shipping Condition	Room temperature (This product is stable at ambient temperature for a few days during ordinary shipping and time spent in Customs)



Solubility Data	
Solubility (In Vitro)	May dissolve in DMSO (in most cases), if not, try other solvents such as H ₂ O, Ethanol, or DMF with a minute amount of products to avoid loss of samples
	Note: Listed below are some common formulations that may be used to formulate products with low water solubility (e.g. < 1 mg/mL), you may test these formulations using a minute amount of products to avoid loss of samples.

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Solubility (In Vivo)	<p style="text-align: center;">Injection Formulations (e.g. IP/IV/IM/SC)</p> <p>Injection Formulation 1: DMSO : Tween 80 □ Saline = 10 : 5 : 85 (i.e. 100 µL DMSO stock solution → 50 µL Tween 80 → 850 µL Saline) *Preparation of saline: Dissolve 0.9 g of sodium chloride in 100 mL ddH₂O to obtain a clear solution.</p> <p>Injection Formulation 2: DMSO : PEG300 □ Tween 80 : Saline = 10 : 40 : 5 : 45 (i.e. 100 µL DMSO → 400 µL PEG300 → 50 µL Tween 80 → 450 µL Saline)</p> <p>Injection Formulation 3: DMSO : Corn oil = 10 : 90 (i.e. 100 µL DMSO → 900 µL Corn oil) Example: Take the Injection Formulation 3 (DMSO : Corn oil = 10 : 90) as an example, if 1 mL of 2.5 mg/mL working solution is to be prepared, you can take 100 µL 25 mg/mL DMSO stock solution and add to 900 µL corn oil, mix well to obtain a clear or suspension solution (2.5 mg/mL, ready for use in animals). ▶ View More ▼</p>
	<p style="text-align: center;">Oral Formulations</p> <p>Oral Formulation 1: Suspend in 0.5% CMC Na (carboxymethylcellulose sodium) Oral Formulation 2: Suspend in 0.5% Carboxymethyl cellulose Example: Take the Oral Formulation 1 (Suspend in 0.5% CMC Na) as an example, if 100 mL of 2.5 mg/mL working solution is to be prepared, you can first prepare 0.5% CMC Na solution by measuring 0.5 g CMC Na and dissolve it in 100 mL ddH₂O to obtain a clear solution; then add 250 mg of the product to 100 mL 0.5% CMC Na solution, to make the suspension solution (2.5 mg/mL, ready for use in animals). ▶ View More ▼</p> <p>Note: Please be aware that the above formulations are for reference only. InvivoChem strongly recommends customers to read literature methods/protocols carefully before determining which formulation you should use for in vivo studies, as different compounds have different solubility properties and have to be formulated differently.</p> <p style="text-align: center;">(Please use freshly prepared in vivo formulations for optimal results.)</p>

Preparing Stock Solutions		1 mg	5 mg	10 mg
	1 mM	6.2016 mL	31.0078 mL	62.0155 mL
	5 mM	1.2403 mL	6.2016 mL	12.4031 mL
	10 mM	0.6202 mL	3.1008 mL	6.2016 mL

***Note:** Please select an appropriate solvent for the preparation of stock solution based on your experiment needs. For most products, DMSO can be used for preparing stock solutions (e.g. 5 mM, 10 mM, or 20 mM concentration); some products with high aqueous solubility may be dissolved in water directly. Solubility information is available at the above Solubility Data section. Once the stock solution is prepared, aliquot it to routine usage volumes and store at -20°C or -80°C. Avoid repeated freeze and thaw cycles.

Biological Activity Assay Protocols (From Reference)	
In Vitro	Drug compounds have included stable heavy isotopes of carbon, hydrogen, and other elements, mostly as quantitative tracers while the drugs were being developed. Because deuteration may have an effect on a drug's pharmacokinetics and metabolic properties, it is a cause for concern [1].
References	[1]. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. Ann Pharmacother. 2019 Feb;53(2):211-216.

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These protocols are for reference only. InvivoChem does not independently validate these methods.

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