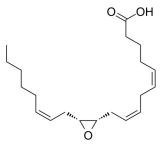
Product Datasheet

Physicochemical Properties



Product Name	(±)11(12)-EET (11,12-EET)
Cat No.	V75164
Molecular Formula	C20H32O3
Molecular Weight	320.46628
Exact Mass	320.235
CAS #	123931-40-8
Related CAS #	(±)11(12)-EET-d11;2699607-19-5
Appearance	Colorless to light yellow liquid
Density	1.0±0.1 g/cm3
Boiling Point	461.8±33.0 °C at 760 mmHg
Flash Point	154.6±18.9 °C
Vapour Pressure	0.0±2.4 mmHg at 25°C
Index of Refraction	1.501
LogP	6.3
tPSA	49.83
Hydrogen Bond Donor Count	1
Hydrogen Bond Acceptor Count	3
Rotatable Bond Count	14
Heavy Atom Count	23
Complexity	396
Defined Atom Stereocenter Count	2
SMILES	CCCCC\C=C\CC1OC1C\C=C\C\C=C\CCCC(O)=O
InChi Key	DXOYQVHGIODESM-LZXKBWHHSA-N
InChi Code	InChI=1S/C20H32O3/c1-2-3-4-5-9-12-15-18-19(23-18)16-13-10-7-6-8-11-14-17-20(21)22/h6,8-10,12-13,18-19H,2-5,7,11,14-17H2,1H3,(H,21,22)/b8-6-,12-9-,13-10-/t18-,19+/m1/s1
Chemical Name	(5Z,8Z)-10-[(2S,3R)-3-[(Z)-oct-2-enyl]oxiran-2-yl]deca-5,8-dienoic acid
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 H2O, 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

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Solubility (In Vivo)	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. **Injection Formulations** **(e.g. IP/IV/IM/SC)** **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 ddH $_2$ O to obtain a clear solution. **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) **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 **Oral Formulations** **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 **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. (Please use freshly prepared in vivo formulations for optimal results.)

Preparing Stock Solutions

Solvent Volume / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	3.1205 mL	15.6023 mL	31.2045 mL
5 mM	0.6241 mL	3.1205 mL	6.2409 mL
10 mM	0.3120 mL	1.5602 mL	3.1205 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 I Assay Protocols (From Reference)

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Targets	NLRP3 inflammasome
In Vitro	In cells and the supernatant, (±)11(12)-EET (5 μM; 10 mimutes; macrophages) significantly lowers the expression of pro-IL-1β, suppresses the production of NLRP3 protein, and lowers intracellular ROS[1].
In vivo	In a container coated with 50 μg/kg of P-selectin and ICAM-1, (±)11(12)-EET promotes the adherence of isolated peripheral blood leukocytes[5].
References	[1]. Epoxyeicosatrienoic acids inhibit the activation of NLRP3 inflammasome in murine macrophages. J Cell Physiol. 2020;235(12):9910-9921. [2]. Novel epoxides formed during the liver cytochrome P-450 oxidation of arachidonic acid. Biochem Biophys Res Commun. 1982;104(3):916-922. [3]. Oxygenation of arachidonic acid by hepatic monooxygenases. Isolation and metabolism of four epoxide intermediates. J Biol Chem. 1982;257(7):3771-3781. [4]. Cytochrome P450 and arachidonic acid bioactivation. Molecular and functional properties of the arachidonate monooxygenase. J Lipid Res. 2000;41(2):163-181. [5]. Arachidonic acid inhibits basolateral K channels in the cortical collecting duct via cytochrome P-450 epoxygenase-dependent metabolic pathways. Am J Physiol Renal Physiol. 2008;294(6):F1441-F1447. [6]. Spector AA. Arachidonic acid cytochrome P450 epoxygenase pathway. J Lipid Res. 2009;50 Suppl(Suppl):S52-S56.

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