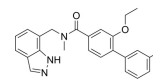


## Product Datasheet

Physicochemical Properties	
Product Name	BAL-0028
Cat No.	V86928
Molecular Formula	C <sub>24</sub> H <sub>22</sub> FN <sub>3</sub> O <sub>2</sub>
Molecular Weight	403.45
CAS #	2842012-69-3
Appearance	White to pink solid powder
Density	1.256±0.06 g/cm <sup>3</sup> (Temp: 20 °C; Press: 760 Torr)(predicted)
Boiling Point	621.6±55.0 °C(predicted)
SMILES	O(C1C=C(C=CC=1C1C=CC=C(C=1)F)C(=O)N(C)CC1C=CC=C2C=NNC=12)CC
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 <sub>2</sub> O, Ethanol, or DMF with a minute amount of products to avoid loss of samples
Solubility (In Vivo)	<p><b>Note:</b> Listed below are some common formulations that may be used to formulate products with low water solubility (e.g. &lt; 1 mg/mL), you may test these formulations using a minute amount of products to avoid loss of samples.</p> <p style="text-align: center;"><b>Injection Formulations</b> (e.g. IP/IV/IM/SC)</p> <p><b>Injection Formulation 1:</b> 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<sub>2</sub>O to obtain a clear solution.</p> <p><b>Injection Formulation 2:</b> 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><b>Injection Formulation 3:</b> DMSO : Corn oil = 10 : 90 (i.e. 100 μL DMSO → 900 μL Corn oil)            Example: Take the <b>Injection Formulation 3</b> (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).  <a href="#">▶ View More ▾</a></p> <p style="text-align: center;"><b>Oral Formulations</b></p> <p><b>Oral Formulation 1:</b> Suspend in 0.5% CMC Na (carboxymethylcellulose sodium)  <b>Oral Formulation 2:</b> Suspend in 0.5% Carboxymethyl cellulose            Example: Take the <b>Oral Formulation 1</b> (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</p>

**Products are for research use only · Not for human or veterinary use**

InvivoChem LLC

Tel: +1 708 310-1919

Fax: +1 708 557-7486

E-mail: [info@invivochem.com](mailto:info@invivochem.com)

<https://www.invivochem.com>

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).

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**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		1 mg	5 mg	10 mg
	1 mM	2.4786 mL	12.3931 mL	24.7862 mL
	5 mM	0.4957 mL	2.4786 mL	4.9572 mL
	10 mM	0.2479 mL	1.2393 mL	2.4786 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.

<b>Biological Activity   Assay Protocols (From Reference)</b>	
Targets	NLRP3 25 nM (IC50)
References	[1]. The discovery of novel and potent indazole NLRP3 inhibitors enabled by DNA-encoded library screening. <i>Bioorg Med Chem Lett.</i> 2024 Feb 28;102:129675.

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

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InvivoChem LLC

Tel: +1 708 310-1919

Fax: +1 708 557-7486

E-mail: [info@invivochem.com](mailto:info@invivochem.com)

<https://www.invivochem.com>