

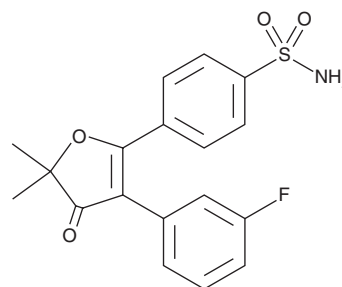
# PRODUCT INFORMATION



## Polmacoxib

Item No. 17509

**CAS Registry No.:** 301692-76-2  
**Formal Name:** 4-[3-(3-fluorophenyl)-4,5-dihydro-5,5-dimethyl-4-oxo-2-furanyl]-benzenesulfonamide  
**MF:** C<sub>18</sub>H<sub>16</sub>FNO<sub>4</sub>S  
**FW:** 361.4  
**Purity:** ≥98%  
**UV/Vis.:** λ<sub>max</sub>: 238, 320 nm  
**Supplied as:** A crystalline solid  
**Storage:** -20°C  
**Stability:** ≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

### Laboratory Procedures

Polmacoxib is supplied as a crystalline solid. A stock solution may be made by dissolving the polmacoxib in the solvent of choice, which should be purged with an inert gas. Polmacoxib is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of polmacoxib in ethanol is approximately 5 mg/ml and approximately 20 mg/ml in DMSO and DMF.

Polmacoxib is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, polmacoxib should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. Polmacoxib has a solubility of approximately 0.5 mg/ml in a 1:8 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

### Description

Polmacoxib is an inhibitor of cyclooxygenase 2 (COX-2) and the carbonic anhydrase subtypes I (CAI) and CAII.<sup>1</sup> It inhibits COX-2 in the absence of carbonic anhydrase II with an IC<sub>50</sub> value of 40 nM, which increases by approximately 4- and 17-fold in the presence of a CAII at a molar ratio of 1:1 and 1:5, respectively.<sup>2</sup> It also inhibits CAI and CAII (IC<sub>50</sub>s = 210 and 95 nM, respectively). Polmacoxib prevents >95 and 90% of prostaglandin E<sub>2</sub> (PGE<sub>2</sub>) production in HCA-7 and HT-29 human colon cancer cells, respectively, using concentrations of 0.01 and 0.001 μg/ml.<sup>3</sup> It inhibits polyp formation in a transgenic mouse model of intestinal polyp formation and tumor growth in human colorectal carcinoma mouse xenograft models when used at a dose of 7 mg/kg. The inhibition of COX-2 and CAII by polmacoxib has the potential for fewer serious systemic adverse effects, including cardiovascular events associated with COX-2 selective inhibitors such as celecoxib (Item No. 10008672).<sup>1,2</sup> Formulations containing polmacoxib have been used in the treatment of osteoarthritis.

### References

1. Singh, O., Kakularam, K.R., Reddanna, P., et al. Understanding the dual inhibition of COX-2 and carbonic anhydrase-II by celecoxib and CG100649 using density functional theory calculations and other molecular modelling approaches. *Protein Pept. Lett.* **22(10)**, 903-912 (2015).
2. Kim, H.T., Cha, H., and Hwang, K.Y. Structural insight into the inhibition of carbonic anhydrase by the COX-2-selective inhibitor polmacoxib (CG100649). *Biochem. Biophys. Res. Commun.* **478(1)**, 1-6 (2016).
3. Kim, S.-H., Margalit, O., Katoh, H., et al. CG100649, a novel COX-2 inhibitor, inhibits colorectal adenoma and carcinoma growth in mouse models. *Invest New Drugs* **32(6)**, 1105-1112 (2014).

#### WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

#### SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

#### WARRANTY AND LIMITATION OF REMEDY

Buyer agrees to purchase the material subject to Cayman's Terms and Conditions. Complete Terms and Conditions including Warranty and Limitation of Liability information can be found on our website.

Copyright Cayman Chemical Company, 11/29/2022

#### CAYMAN CHEMICAL

1180 EAST ELLSWORTH RD  
ANN ARBOR, MI 48108 · USA

PHONE: [800] 364-9897

[734] 971-3335

FAX: [734] 971-3640

CUSTSERV@CAYMANCHEM.COM

WWW.CAYMANCHEM.COM