

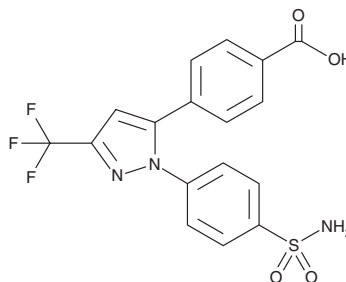
PRODUCT INFORMATION



Celecoxib Carboxylic Acid

Item No. 34062

CAS Registry No.: 170571-01-4
Formal Name: 4-[1-[4-(aminosulfonyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]-benzoic acid
MF: C₁₇H₁₂F₃N₃O₄S
FW: 411.4
Purity: ≥95%
Supplied as: A 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

Celecoxib carboxylic acid is supplied as a solid. A stock solution may be made by dissolving the celecoxib carboxylic acid in the solvent of choice, which should be purged with an inert gas. Celecoxib carboxylic acid is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide. The solubility of celecoxib carboxylic acid in these solvents is approximately 30 mg/ml. Celecoxib carboxylic acid is slightly soluble in PBS (pH 7.2).

Celecoxib carboxylic acid is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, celecoxib carboxylic acid should first be dissolved in ethanol and then diluted with the aqueous buffer of choice. Celecoxib carboxylic acid has a solubility of approximately 0.12 mg/ml in a 1:6 solution of ethanol:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

Celecoxib carboxylic acid is an inactive metabolite of the COX-2 inhibitor celecoxib (Item No. 10008672).^{1,2} It is formed from celecoxib primarily by the cytochrome P450 (CYP) isoform CYP2C9.

References

1. Liu, H., Huang, X., Shen, J., *et al.* Inhibitory mode of 1,5-diarylpyrazole derivatives against cyclooxygenase-2 and cyclooxygenase-1: Molecular docking and 3D QSAR analyses. *J. Med. Chem.* **45(22)**, 4816-4827 (2002).
2. Kim, S.-H., Kim, D.-H., Byeon, J.-Y., *et al.* Effects of CYP2C9 genetic polymorphisms on the pharmacokinetics of celecoxib and its carboxylic acid metabolite. *Arch. Pharm. Res.* **40(3)**, 382-390 (2017).

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.

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