CD BioGlyco

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# Product Information

## AhR inhibitor, ITE, Purity ≥98%

**Cat. No.:** X24-09-YM448

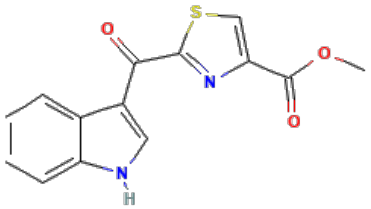
**Size:** 5 mg; 10 mg; 50 mg; 100 mg

**MDL:** MFCD06411597

**CAS Number:** 448906-42-1

**Compound CID:** 4668801

**Synonym:** 448906-42-1; 2-[1*H*-Indol-3-yl(oxo)methyl]-4-thiazolecarboxylic acid methyl ester; Methyl 2-(1*H*-indole-3-carbonyl)-1,3-thiazole-4-carboxylate; AhR inhibitor



**This product is for research use only and is not intended for diagnostic use.**

## Product Information

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| **Description** | ITE is an effective metabolism inhibitor, that has the ability to prevent the pathway of cell metabolism by inhibiting AhR. The molecular weight of the compound is 286.31, and its molecular formula is $C_{14}H_{10}N_2O_3S$. |
| **Molecular Weight** | 286.31 |
| **Molecular Formula** | $C_{14}H_{10}N_2O_3S$ |
| **IUPAC Name** | Methyl 2-(1*H*-indole-3-carbonyl)-1,3-thiazole-4-carboxylate |
| **InChI** | InChI=1S/C14H10N2O3S/c1-19-14(18)11-7-20-13(16-11)12(17)9-6-15-10-5-3-2-4-8(9)10/h2-7,15H,1H3 |
| **InChI Key** | KDDXOGDIPZSCTM-UHFFFAOYSA-N |
| **Canonical SMILES** | COC(=O)C1=CSC(=N1)C(=O)C2=CNC3=CC=CC=C32 |
| **Isomeric SMILES** | COC1=C(C2=C3[C@H](CC4=CC(=C(C=C42)OC)O)NCCC3=C1)O |
| **Form** | Lyophilized powder |
| **Purity** | ≥98% |
| **Impurities** | Free from inappropriate visible particulates, foreign matter, discoloration, or other defects. |
| **Identity** | Confirmed by NMR/HPLC/MS. |
| **Stability** | In its lyophilized form, the chemical remains stable for 36 months. |
| **Quality Level** | Research grade |
| **Applications** | ITE displays the significant potential to act as an effective endogenous agonist of aryl hydrocarbon receptor (AhR), binding directly to AHR, with a Ki of 3 nM. |

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| **Storage** | Store at -20ºC, and keep desiccated. |