

# [Epacadostat c11h13brfn7o4s structure](https://assignbuster.com/epacadostat-c11h13brfn7o4s-structure/)

Contents

* Bio Activity:

|  |  |
| --- | --- |
| Molecular Formula | C 11 H 13 BrFN 7 O 4 S |
| Average mass | 438. 233 Da |
| Density | 2. 0±0. 1 g/cm 3 |
| Boiling Point | 672. 3±65. 0 °C at 760 mmHg |
| Flash Point | 360. 4±34. 3 °C |
| Molar Refractivity | 87. 8±0. 5 cm 3 |
| Polarizability | 34. 8±0. 5 10 -24 cm 3 |
| Surface Tension | 77. 6±7. 0 dyne/cm |
| Molar Volume | 217. 3±7. 0 cm 3 |

* Experimental data
* Predicted – ACD/Labs
* Predicted – ChemAxon
* Experimental Physico-chemical Properties

## Experimental Solubility:

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| --- |
| DMSO 50 mg/mlMedChem ExpressHY-15689 |
| Soluble in DMSOAxon Medchem1733 |
| Water 100 mM MethanolMedChem ExpressHY-15689 |

* Miscellaneous

## Safety:

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| --- |
| 5Axon Medchem1733 |
| H303; H313; H317; H333; H334; H335; H373Axon Medchem1733 |
| no pictogramAxon Medchem1733 |
| P101; P102; P103; P260; P262; P263; P264; P270; P280; P304; P312; P340Axon Medchem1733 |
| WarningAxon Medchem1733 |

## Bio Activity:

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| IDOMedChem ExpressHY-15689 |
| INCB 024360 is a potent and novel indoleamine-2, 3 dioxygenase (IDO)inhibitor with an IC50 value <100 nM. MedChem Express |
| INCB 024360 is a potent and novel indoleamine-2, 3 dioxygenase (IDO)inhibitor with an IC50 value <100 nM.; IC50 Value: <100 nM [1]; Target: Indoleamine-2, 3-dioxygenase ; IDO is an immunomodulatory enzyme produced by some alternatively activated macrophages and other immunoregulatory cells (also used as an immune subversion strategy by many tumors). MedChem ExpressHY-15689 |
| INCB 024360 is a potent and novel indoleamine-2, 3 dioxygenase (IDO)inhibitor with an IC50 value <100 nM.; IC50 Value: <100 nM [1]; Target: Indoleamine-2, 3-dioxygenase ; IDO is an immunomodulatory enzyme produced by some alternatively activated macrophages and other immunoregulatory cells (also used as an immune subversion strategy by many tumors). Interferon-gamma has an antiproliferative effect on many tumor cells and inhibits intracellular pathogens such as Toxoplasma and chlamydia, at least partly because of the induction of indoleamine 2, 3-dioxygenase. MedChem ExpressHY-15689 |
| Metabolic Enzyme/Protease; MedChem ExpressHY-15689 |
| OthersMedChem ExpressHY-15689 |

Predicted data is generated using the ACD/Labs Percepta Platform – PhysChem Module

|  |  |
| --- | --- |
| Density: | 2. 0±0. 1 g/cm 3 |
| Boiling Point: | 672. 3±65. 0 °C at 760 mmHg |
| Vapour Pressure: | 0. 0±2. 2 mmHg at 25°C |
| Enthalpy of Vaporization: | 103. 7±3. 0 kJ/mol |
| Flash Point: | 360. 4±34. 3 °C |
| Index of Refraction: | 1. 742 |
| Molar Refractivity: | 87. 8±0. 5 cm 3 |
| #H bond acceptors: | 11 |
| #H bond donors: | 6 |
| #Freely Rotating Bonds: | 8 |
| #Rule of 5 Violations: | 2 |

|  |  |
| --- | --- |
| ACD/LogP: | 3. 92 |
| ACD/LogD (pH 5. 5): | 1. 99 |
| ACD/BCF (pH 5. 5): | 19. 27 |
| ACD/KOC (pH 5. 5): | 289. 16 |
| ACD/LogD (pH 7. 4): | 1. 99 |
| ACD/BCF (pH 7. 4): | 19. 26 |
| ACD/KOC (pH 7. 4): | 288. 98 |
| Polar Surface Area: | 176 Å 2 |
| Polarizability: | 34. 8±0. 5 10 -24 cm 3 |
| Surface Tension: | 77. 6±7. 0 dyne/cm |
| Molar Volume: | 217. 3±7. 0 cm 3 |

Click to predict properties on the Chemicalize site