

# [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:

|  |
| --- |
| 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

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| --- | --- |
| 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  |

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| --- | --- |
| 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