

# [Apalutamide c21h15f4n5o2s structure](https://assignbuster.com/apalutamide-c21h15f4n5o2s-structure/)

Contents

* Bio Activity:

|  |  |
| --- | --- |
| Molecular Formula  | C 21 H 15 F 4 N 5 O 2 S  |
| Average mass  | 477. 435 Da  |
| Density  | 1. 6±0. 1 g/cm 3  |
| Boiling Point  |  |
| Flash Point  |  |
| Molar Refractivity  | 110. 7±0. 4 cm 3  |
| Polarizability  | 43. 9±0. 5 10 -24 cm 3  |
| Surface Tension  | 75. 2±5. 0 dyne/cm  |
| Molar Volume  | 300. 2±5. 0 cm 3  |

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

## Experimental Solubility:

|  |
| --- |
| DMSO 15 mg/mL Ethanol 5 mg/mLMedChem ExpressHY-16060  |
| Soluble in DMSOAxon Medchem1979  |

* Miscellaneous

## Safety:

|  |
| --- |
| 5Axon Medchem1979  |
| H303; H313; H317; H333; H334; H335; H373Axon Medchem1979  |
| no pictogramAxon Medchem1979  |
| P101; P102; P103; P260; P262; P263; P264; P270; P280; P304; P312; P340Axon Medchem1979  |
| WarningAxon Medchem1979  |

## Target Organs:

|  |
| --- |
| Androgen Receptor inhibitorTargetMolT2339  |

## Bio Activity:

|  |
| --- |
| Androgen ReceptorMedChem ExpressHY-16060  |
| Androgen Receptor; GABAA receptorTargetMolT2339  |
| ARN-509 is a selective and competitive androgen receptor inhibitor with IC50 of 16 nM, useful for prostate cancer treatment. MedChem Express  |
| ARN-509 is a selective and competitive androgen receptor inhibitor with IC50 of 16 nM, useful for prostate cancer treatment.; IC50 value: 16 nM; Target: androgen receptorARN-509 is an androgen receptor antagonist with potential antineoplastic activity. ARN-509 binds to AR in target tissues thereby preventing androgen-induced receptor activation and facilitating the formation of inactive complexes that cannot be translocated to the nucleus. This prevents binding to and transcription of AR-responsive genes. This ultimately inhibits the expression of genes that regulate prostate cancer cell proliferation and may lead to an inhibition of cell growth in AR-expressing tumor cells. MedChem ExpressHY-16060  |
| Endocrinology/ HormonesTargetMolT2339  |

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

|  |  |
| --- | --- |
| Density:  | 1. 6±0. 1 g/cm 3  |
| Boiling Point:  |  |
| Vapour Pressure:  |  |
| Enthalpy of Vaporization:  |  |
| Flash Point:  |  |
| Index of Refraction:  | 1. 659  |
| Molar Refractivity:  | 110. 7±0. 4 cm 3  |
| #H bond acceptors:  | 7  |
| #H bond donors:  | 1  |
| #Freely Rotating Bonds:  | 5  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 1. 30  |
| ACD/LogD (pH 5. 5):  | 1. 38  |
| ACD/BCF (pH 5. 5):  | 6. 54  |
| ACD/KOC (pH 5. 5):  | 133. 48  |
| ACD/LogD (pH 7. 4):  | 1. 38  |
| ACD/BCF (pH 7. 4):  | 6. 54  |
| ACD/KOC (pH 7. 4):  | 133. 48  |
| Polar Surface Area:  | 121 Å 2  |
| Polarizability:  | 43. 9±0. 5 10 -24 cm 3  |
| Surface Tension:  | 75. 2±5. 0 dyne/cm  |
| Molar Volume:  | 300. 2±5. 0 cm 3  |

Click to predict properties on the Chemicalize site