

# [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:

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| --- |
| 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:

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| --- |
| Androgen Receptor inhibitorTargetMolT2339 |

## Bio Activity:

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| --- |
| 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