

Apalutamide  
c<sub>21</sub>h<sub>15</sub>f<sub>4</sub>n<sub>5</sub>o<sub>2</sub>s  
structure



## Contents

- Bio Activity:

Molecular      C<sub>21</sub> H<sub>15</sub> F<sub>4</sub> N<sub>5</sub>

Formula        O<sub>2</sub> S

Average mass 477. 435 Da

Density        1. 6±0. 1 g/cm<sup>3</sup>

Boiling Point

Flash Point

Molar  
Refractivity    110. 7±0. 4 cm<sup>3</sup>

Polarizability    43. 9±0. 5 10<sup>-24</sup>  
cm<sup>3</sup>

Surface        75. 2±5. 0

Tension        dyne/cm

Molar Volume 300. 2±5. 0 cm<sup>3</sup>

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

- **Experimental Solubility:**

DMSO 15 mg/mL

Ethanol 5

mg/mL MedChem

ExpressHY-16060

Soluble in

DMSO Axon

Medchem1979

- Miscellaneous

- **Safety:**

5 Axon

Medchem1979

H303; H313; H317;

H333; H334; H335;

H373 Axon

Medchem1979

no pictogram Axon

Medchem1979

P101; P102; P103;

P260; P262; P263;

P264; P270; P280;

P304; P312;

P340Axon

Medchem1979

WarningAxon

Medchem1979

- **Target Organs:**

Androgen Receptor

inhibitorTargetMolT2

339

- **Bio Activity:**

Androgen

ReceptorMedChem

ExpressHY-16060

Androgen Receptor;

GABAA

receptorTargetMolT2

339

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

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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/  
HormonesTargetMol  
T2339

Density: 1.6±0.1 g/cm<sup>3</sup>

Boiling Point:

Vapour Pressure:

Enthalpy of Vaporization:

Flash Point:

Index of Refraction: 1.659

Molar Refractivity: 110.7±0.4 cm<sup>3</sup>

#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 <sup>2</sup>
Polarizability:	43.9 ± 0.5 10 <sup>-24</sup> cm <sup>3</sup>
Surface Tension:	75.2 ± 5.0 dyne/cm
Molar Volume:	300.2 ± 5.0 cm <sup>3</sup>

Click to predict properties on the Chemicalize site