Umifenovir hydrochloride c22h26brcln2o3s structure



Contents

Bio Activity:		
Molecular	C ₂₂ H ₂₆ BrClN ₂	
Formula	O 3 S	
Average mass	513. 875 Da	
Density		
Boiling Point		
Flash Point		
Molar		
Refractivity		
Polarizability		
Surface		
Tension		
Molar Volume		
• Eynerime	ental data	

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

• Experimental Melting Point:

133 °CBiosynthJ-

501287

133-137 °C

(Decomposes)LabNet

workLN00191929

• Experimental Solubility:

DMSO 48

mg/mlMedChem

ExpressHY-14904A

in DMSO > 10

mMMedChem

ExpressHY-14904A

Miscellaneous

• Safety:

IRRITANTMatrix

Scientific092967

• Bio Activity:

Anti-

infectionMedChem

ExpressHY-14904A

Anti-infection;

MedChem

ExpressHY-14904A

Arbidol (Umifenovir)

hydrochloride is an

broad-spectrum

antiviral chemical

agent which can

inhibit cell entry of

enveloped viruses by

blocking viral fusion

with host cell

membraneMedChem

Express

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https://assignbuster.com/umifenovir-hydrochloride-c22h26brcln2o3s-structure/

membrane; IC50

value:; Target:

Antiviral; Anti-

influenza agent; in

vitro: Arbidol was

found to present

potent inhibitory

activity against

enveloped and non-

enveloped RNA

viruses, including

FLU-A, RSV, HRV 14

and CVB3 when

added before, during,

or after viral

infection, with 50%

inhibitory

concentration (IC50)

ranging from 2.7 to

13. 8 microg/ml.

However, arbidol

showed selective

antiviral activity

against AdV-7, a DNA

virus, only when

added after infection

(therapeutic index

(TI) = 5.5)[1].

MedChem

ExpressHY-14904A

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interacts with the

polar head-group of

phospholipid at the

membrane interface.

Fluorescence studies

of interactions

between Arb and

either tryptophan

derivatives or

	membrane peptides		
	reconstituted into		
	liposomes show that		
	Arb interacts with		
	tryptophan in the		
	micromolar range.		
	Interestingly,		
	apparent binding		
	affinities between		
	IMedChem		
	ExpressHY-14904A		
	Influenza		
	VirusMedChem		
	ExpressHY-14904A		
Predicted d	lata is generated using the ACD/Labs Percepta Platform -		
PhysChem	Module		
No predicte	ed properties have been calculated for this compound.		
Density:			
Boiling Poir	nt:		
Vapour Pressure:			

https://assignbuster.com/umifenovir-hydrochloride-c22h26brcln2o3s-structure/

Enthalpy of Vaporization:
Flash Point:
Index of Refraction:
Molar Refractivity:
#H bond acceptors:
#H bond donors:
#Freely Rotating Bonds:
#Rule of 5 Violations:
ACD/LogP:
ACD/LogD (pH 5. 5):
ACD/BCF (pH 5. 5):
ACD/KOC (pH 5. 5):
ACD/LogD (pH 7. 4):
ACD/BCF (pH 7. 4):
ACD/KOC (pH 7. 4):

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Polar Surface Area:	
Polarizability:	
Surface Tension:	

Click to predict properties on the Chemicalize site

Molar Volume: