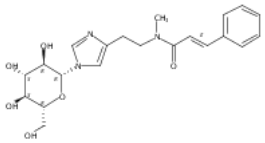
Score: 87

1.

5853-02-1



Double bond geometry as shown., Absolute stereochemistry.

C_{21} H_{27} N_3 O_6
2-Propenamide, *N*-[2-(1-β-D-glucopyranosyl-1*H*-imidazol-4-yl)ethyl]-*N*-methyl-3-phenyl-, (2*E*)-

Key Physical Properties:

Molecular Weight
417.46
Melting Point (Experimental)
Value: 226.5-228.0 °C
Boiling Point (Predicted)
Value: 777.8±60.0 °C | Condition: Press: 760 Torr
Density (Predicted)
Value: 1.37±0.1 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr
pKa (Predicted)
Value: 13.13±0.70 | Condition: Most Acidic Temp: 25 °C

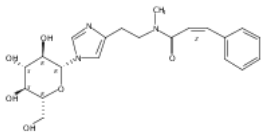
Related Info:

~ 12 References
~ 2 Commercial Sources
Spectra
Experimental Properties

Score: 87

2.

51013-83-3



Double bond geometry as shown., Absolute stereochemistry.

C_{21} H_{27} N_3 O_6
2-Propenamide, *N*-[2-(1-β-D-glucopyranosyl-1*H*-imidazol-4-yl)ethyl]-*N*-methyl-3-phenyl-, (*Z*)-(9CI)

Key Physical Properties:

Molecular Weight
417.46
Boiling Point (Predicted)
Value: 777.8±60.0 °C | Condition: Press: 760 Torr
Density (Predicted)
Value: 1.37±0.1 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr
pKa (Predicted)
Value: 13.13±0.70 | Condition: Most Acidic Temp: 25 °C

Related Info:

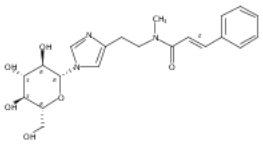
~ 1 References

Score: 87

3.

119659-36-8

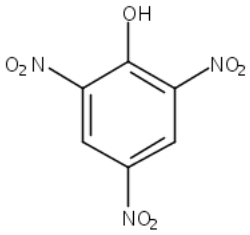
5853-02-1
C_{21} H_{27} N_3 O_6



Double bond geometry as shown.,

Absolute stereochemistry.

88-89-1
C_6 H_3 N_3 O_7



C_{21} H_{27} N_3 O_6 . C_6 H_3 N_3 O_7
Casimiroedine, picrate (6CI)

Key Physical Properties:

Melting Point (Experimental)
Value: 110-112 °C | Condition: Solv: methanol (67-56-1)

Related Info:

~ 1 References
Experimental Properties