SMILES: 00

Molecular Formula: H<sub>2</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 18.635 ± 3.070

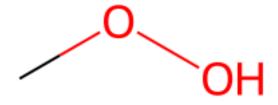


## **Molecule 2**

SMILES: COO

Molecular Formula: CH<sub>4</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 18.615 ± 4.150



# **Molecule 3**

SMILES: OCO

Molecular Formula: CH<sub>4</sub>O<sub>2</sub>

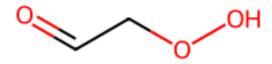
Predicted Column Density ( $log_{10} cm^{-2}$ ): 18.125 ± 3.096



SMILES: O=CCOO

Molecular Formula: C<sub>2</sub>H<sub>4</sub>O<sub>3</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 17.449 ± 4.991

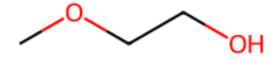


## **Molecule 5**

**SMILES: COCCO** 

Molecular Formula: C<sub>3</sub>H<sub>8</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 17.415 ± 4.603



# **Molecule 6**

SMILES: CC

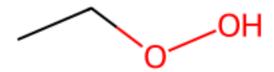
Molecular Formula: C<sub>2</sub>H<sub>6</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 17.239 ± 3.012

SMILES: CCOO

Molecular Formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 17.198 ± 4.807

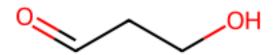


## **Molecule 8**

SMILES: O=CCCO

Molecular Formula: C<sub>3</sub>H<sub>6</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 17.071 ± 4.617



# **Molecule 9**

SMILES: O=C=O

Molecular Formula: CO2

Predicted Column Density ( $log_{10} cm^{-2}$ ): 17.057 ± 3.431



SMILES: S=C=S

Molecular Formula: CS2

Predicted Column Density ( $log_{10} cm^{-2}$ ): 17.022 ± 4.500



### **Molecule 11**

**SMILES: COCOC** 

Molecular Formula: C<sub>3</sub>H<sub>8</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.963 ± 3.805



# **Molecule 12**

SMILES: CN

Molecular Formula: CH<sub>5</sub>N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.925 ± 2.141



SMILES: COC=C=O

 $Molecular\ Formula:\ C_3H_4O_2$ 

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.901 ± 3.685

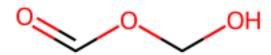


## **Molecule 14**

SMILES: O=COCO

Molecular Formula: C<sub>2</sub>H<sub>4</sub>O<sub>3</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.870 ± 3.920

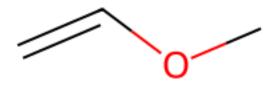


# **Molecule 15**

SMILES: C=COC

Molecular Formula: C₃H<sub>6</sub>O

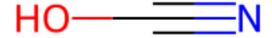
Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.783 ± 3.033



SMILES: N#CO

Molecular Formula: CHNO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.740 ± 3.977

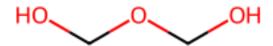


### **Molecule 17**

**SMILES: OCOCO** 

Molecular Formula: C<sub>2</sub>H<sub>6</sub>O<sub>3</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.694 ± 4.465

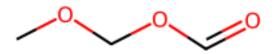


# **Molecule 18**

SMILES: COCOC=0

Molecular Formula: C<sub>3</sub>H<sub>6</sub>O<sub>3</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.614 ± 4.878



SMILES: C=C

Molecular Formula: C<sub>2</sub>H<sub>4</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.589 ± 2.459

#### **Molecule 20**

SMILES: CC=COC

Molecular Formula: C<sub>4</sub>H<sub>8</sub>O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.552 ± 4.344

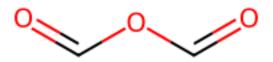


# **Molecule 21**

SMILES: O=COC=O

Molecular Formula: C<sub>2</sub>H<sub>2</sub>O<sub>3</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.503 ± 4.755



SMILES: C#C

Molecular Formula: C<sub>2</sub>H<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.499 ± 4.726

# **Molecule 23**

SMILES: COCC=O

Molecular Formula: C<sub>3</sub>H<sub>6</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.492 ± 3.608

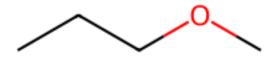


# **Molecule 24**

SMILES: CCCOC

Molecular Formula:  $C_4H_{10}O$ 

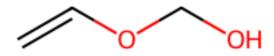
Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.489 ± 4.413



SMILES: C=COCO

Molecular Formula: C₃H<sub>6</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.385 ± 4.725



## **Molecule 26**

SMILES: O=C=C=O

Molecular Formula: C<sub>2</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.369 ± 4.652

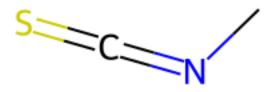


### **Molecule 27**

SMILES: CN=C=S

 $Molecular\ Formula:\ C_2H_3NS$ 

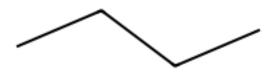
Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.337 ± 4.034



SMILES: CCCC

Molecular Formula: C<sub>4</sub>H<sub>10</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.332 ± 4.622

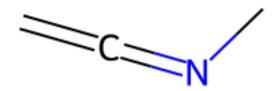


#### **Molecule 29**

SMILES: C=C=NC

Molecular Formula: C<sub>3</sub>H<sub>5</sub>N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.296 ± 4.195

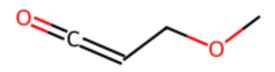


# **Molecule 30**

SMILES: COCC=C=O

Molecular Formula: C<sub>4</sub>H<sub>6</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.293 ± 4.786



SMILES: N#N

Molecular Formula: N2

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.286 ± 3.030



## **Molecule 32**

SMILES: COC=CC=O

Molecular Formula: C<sub>4</sub>H<sub>6</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.282 ± 3.672



# **Molecule 33**

SMILES: C=C=C

Molecular Formula: C₃H₄

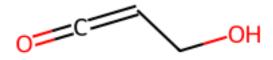
Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.257 ± 3.652



SMILES: O=C=CCO

Molecular Formula: C<sub>3</sub>H<sub>4</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.254 ± 3.589

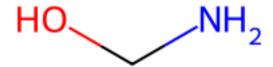


## **Molecule 35**

SMILES: NCO

Molecular Formula: CH₅NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.221 ± 4.076



# **Molecule 36**

SMILES: CCCC=O

Molecular Formula:  $C_4H_8O$ 

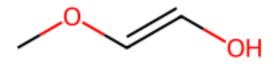
Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.144 ± 4.904



SMILES: COC=CO

Molecular Formula: C₃H<sub>6</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.127 ± 4.157

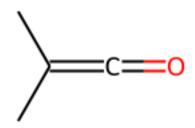


## **Molecule 38**

SMILES: CC(C)=C=O

Molecular Formula: C<sub>4</sub>H<sub>6</sub>O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.080 ± 4.778



# **Molecule 39**

SMILES: O=C=C=S

Molecular Formula: C<sub>2</sub>OS

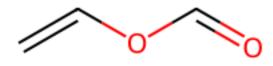
Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.063 ± 3.431



SMILES: C=COC=O

 $Molecular\ Formula:\ C_3H_4O_2$ 

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.018 ± 4.947

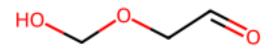


## **Molecule 41**

SMILES: O=CCOCO

Molecular Formula: C<sub>3</sub>H<sub>6</sub>O<sub>3</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.967 ± 4.996



# **Molecule 42**

SMILES: COC#N

Molecular Formula: C<sub>2</sub>H<sub>3</sub>NO

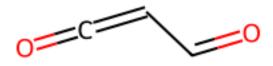
Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.951 ± 4.028



SMILES: O=C=CC=O

Molecular Formula: C₃H₂O₂

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.930 ± 3.325

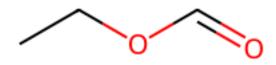


## **Molecule 44**

SMILES: CCOC=O

Molecular Formula: C<sub>3</sub>H<sub>6</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.892 ± 3.853

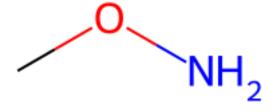


# **Molecule 45**

SMILES: CON

Molecular Formula: CH₅NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.878 ± 4.513



SMILES: O=CC=O

Molecular Formula: C<sub>2</sub>H<sub>2</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.857 ± 3.120

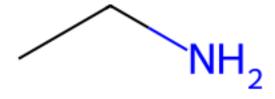


## **Molecule 47**

SMILES: CCN

Molecular Formula: C<sub>2</sub>H<sub>7</sub>N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.835 ± 3.730



## **Molecule 48**

SMILES: C=C=N

Molecular Formula: C<sub>2</sub>H<sub>3</sub>N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.825 ± 3.850



SMILES: OS

Molecular Formula: H₂OS

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.811 ± 2.851



#### **Molecule 50**

**SMILES: COCN** 

Molecular Formula: C<sub>2</sub>H<sub>7</sub>NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.772 ± 4.388



# **Molecule 51**

SMILES: S=C=C=S

Molecular Formula: C<sub>2</sub>S<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.757 ± 4.928



SMILES: C1COCO1

Molecular Formula: C₃H<sub>6</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.741 ± 4.389

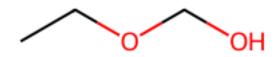


## **Molecule 53**

**SMILES: CCOCO** 

Molecular Formula: C<sub>3</sub>H<sub>8</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.716 ± 3.731

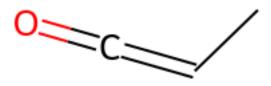


# **Molecule 54**

SMILES: CC=C=O

Molecular Formula: C₃H₄O

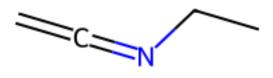
Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.690 ± 3.755



SMILES: C=C=NCC

Molecular Formula: C<sub>4</sub>H<sub>7</sub>N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.665 ± 4.872

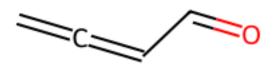


## **Molecule 56**

SMILES: C=C=CC=O

Molecular Formula: C<sub>4</sub>H<sub>4</sub>O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.652 ± 3.853

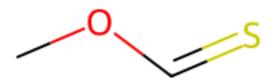


# **Molecule 57**

SMILES: COC=S

Molecular Formula: C<sub>2</sub>H<sub>4</sub>OS

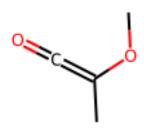
Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.652 ± 4.065



SMILES: COC(C)=C=O

Molecular Formula: C<sub>4</sub>H<sub>6</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.609 ± 4.279

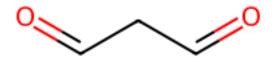


## **Molecule 59**

SMILES: O=CCC=O

Molecular Formula: C<sub>3</sub>H<sub>4</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.599  $\pm$  4.504



# **Molecule 60**

SMILES: O=C=NCO

Molecular Formula: C<sub>2</sub>H<sub>3</sub>NO<sub>2</sub>

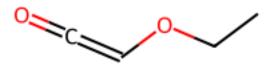
Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.557 ± 3.939

0 C N OH

SMILES: CCOC=C=O

Molecular Formula: C<sub>4</sub>H<sub>6</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.526 ± 4.589

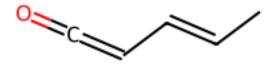


## **Molecule 62**

SMILES: CC=CC=C=O

Molecular Formula: C₅H6O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.467 ± 4.629

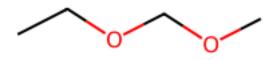


# **Molecule 63**

SMILES: CCOCOC

Molecular Formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>

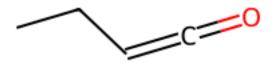
Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.460 ± 4.958



SMILES: CCC=C=O

Molecular Formula: C<sub>4</sub>H<sub>6</sub>O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.458 ± 4.136

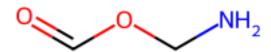


#### **Molecule 65**

SMILES: NCOC=O

Molecular Formula: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.423 ± 4.881

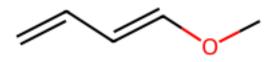


# **Molecule 66**

SMILES: C=CC=COC

Molecular Formula: C₅H<sub>8</sub>O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.420 ± 4.710



SMILES: C=CCOC

Molecular Formula: C<sub>4</sub>H<sub>8</sub>O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.417 ± 4.431



## **Molecule 68**

SMILES: NN

Molecular Formula: H<sub>4</sub>N<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.416 ± 3.019

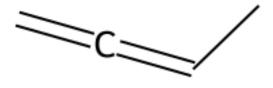
$$H_2N$$
— $NH_2$ 

# **Molecule 69**

SMILES: C=C=CC

Molecular Formula: C<sub>4</sub>H<sub>6</sub>

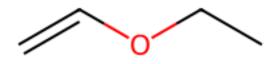
Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.412 ± 4.954



SMILES: C=COCC

Molecular Formula: C<sub>4</sub>H<sub>8</sub>O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.407 ± 4.334

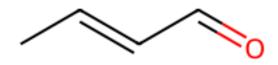


## **Molecule 71**

SMILES: CC=CC=O

Molecular Formula: C<sub>4</sub>H<sub>6</sub>O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.394 ± 3.339

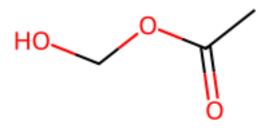


# **Molecule 72**

SMILES: CC(=0)OCO

Molecular Formula: C₃H<sub>6</sub>O<sub>3</sub>

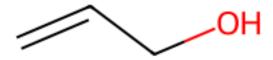
Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.390 ± 4.387



SMILES: C=CCO

Molecular Formula: C₃H<sub>6</sub>O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.378 ± 3.164

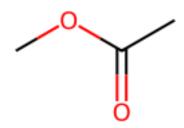


## **Molecule 74**

SMILES: COC(C)=O

Molecular Formula: C<sub>3</sub>H<sub>6</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.328 ± 3.065



### **Molecule 75**

SMILES: C#[SH]

Molecular Formula: CH<sub>2</sub>S

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.324 ± 3.131



SMILES: CC(C)=S

Molecular Formula: C₃H<sub>6</sub>S

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.289 ± 4.309



## **Molecule 77**

SMILES: N#CCO

Molecular Formula: C<sub>2</sub>H<sub>3</sub>NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.288 ± 3.144

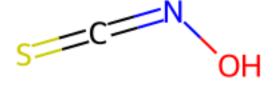


# **Molecule 78**

SMILES: ON=C=S

Molecular Formula: CHNOS

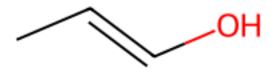
Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.270 ± 4.688



SMILES: CC=CO

Molecular Formula: C₃H<sub>6</sub>O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.239 ± 4.093

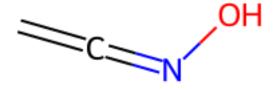


## **Molecule 80**

SMILES: C=C=NO

Molecular Formula: C<sub>2</sub>H<sub>3</sub>NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.228 ± 4.872



# **Molecule 81**

SMILES: C=C=C=O

Molecular Formula: C₃H₂O

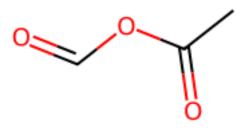
Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.223 ± 4.020



SMILES: CC(=0)OC=0

Molecular Formula: C<sub>3</sub>H<sub>4</sub>O<sub>3</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.217 ± 4.514

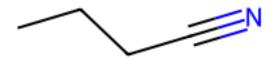


## **Molecule 83**

SMILES: CCCC#N

Molecular Formula: C<sub>4</sub>H<sub>7</sub>N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.200 ± 4.879

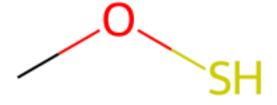


# **Molecule 84**

SMILES: COS

Molecular Formula: CH₄OS

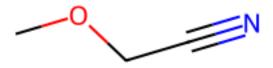
Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.184 ± 4.029



SMILES: COCC#N

Molecular Formula: C₃H₅NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.182 ± 3.559

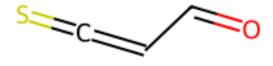


## **Molecule 86**

SMILES: O=CC=C=S

Molecular Formula: C<sub>3</sub>H<sub>2</sub>OS

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.151 ± 3.984

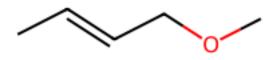


# **Molecule 87**

SMILES: CC=CCOC

Molecular Formula: C5H10O

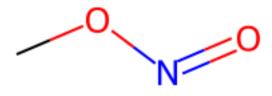
Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.136 ± 4.648



SMILES: CON=O

Molecular Formula: CH₃NO2

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.134 ± 3.776

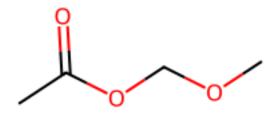


## **Molecule 89**

SMILES: COCOC(C)=0

Molecular Formula: C<sub>4</sub>H<sub>8</sub>O<sub>3</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.134 ± 4.824

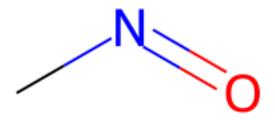


# **Molecule 90**

SMILES: CN=O

Molecular Formula: CH₃NO

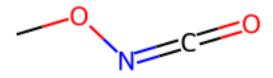
Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.131 ± 3.894



SMILES: CON=C=O

Molecular Formula: C<sub>2</sub>H<sub>3</sub>NO<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.129 ± 4.696

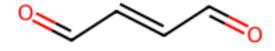


## **Molecule 92**

SMILES: O=CC=CC=O

Molecular Formula: C<sub>4</sub>H<sub>4</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.124 ± 4.006

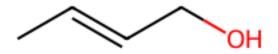


# **Molecule 93**

SMILES: CC=CCO

Molecular Formula: C<sub>4</sub>H<sub>8</sub>O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.098 ± 4.185



SMILES: N=C=N

Molecular Formula: CH<sub>2</sub>N<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.083 ± 4.708

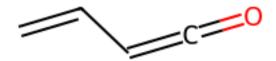


#### **Molecule 95**

SMILES: C=CC=C=O

Molecular Formula: C<sub>4</sub>H<sub>4</sub>O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.067 ± 3.364

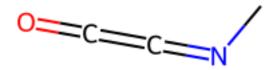


### **Molecule 96**

SMILES: CN=C=C=O

Molecular Formula: C₃H₃NO

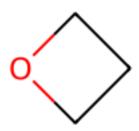
Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.061 ± 4.445



SMILES: C1COC1

Molecular Formula: C<sub>3</sub>H<sub>6</sub>O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.058 ± 3.241



### **Molecule 98**

SMILES: N#CC=O

Molecular Formula: C2HNO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.041 ± 3.444

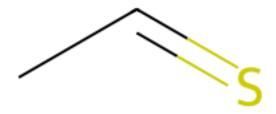


# **Molecule 99**

SMILES: CC=S

Molecular Formula: C<sub>2</sub>H<sub>4</sub>S

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.035 ± 3.778



SMILES: COC=S=O

Molecular Formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>S

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.023 ± 4.614

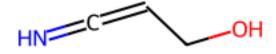


## **Molecule 101**

SMILES: N=C=CCO

Molecular Formula: C<sub>3</sub>H<sub>5</sub>NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.999 ± 4.909

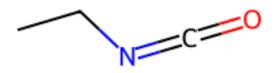


# **Molecule 102**

SMILES: CCN=C=O

Molecular Formula: C₃H₅NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.930 ± 3.889



SMILES: C=C=C=S

Molecular Formula: C₃H₂S

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.918 ± 4.675

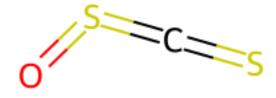


## **Molecule 104**

SMILES: O=S=C=S

Molecular Formula: COS<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.913 ± 4.013

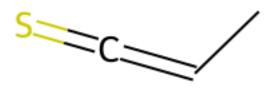


# **Molecule 105**

SMILES: CC=C=S

Molecular Formula: C₃H₄S

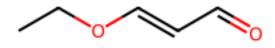
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.910 ± 4.650



SMILES: CCOC=CC=O

Molecular Formula: C₅H<sub>8</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.907 ± 4.845



# **Molecule 107**

SMILES: O=C=S=O

Molecular Formula: CO<sub>2</sub>S

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.893 ± 4.113



# **Molecule 108**

SMILES: N=C=C=O

Molecular Formula: C₂HNO

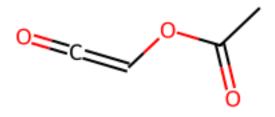
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.867 ± 4.030



SMILES: CC(=O)OC=C=O

Molecular Formula: C<sub>4</sub>H<sub>4</sub>O<sub>3</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.851 ± 4.820

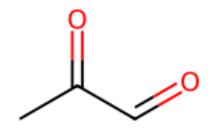


## **Molecule 110**

SMILES: CC(=O)C=O

Molecular Formula: C<sub>3</sub>H<sub>4</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.839 ± 4.573

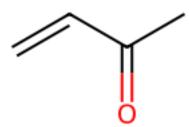


## **Molecule 111**

SMILES: C=CC(C)=O

Molecular Formula: C<sub>4</sub>H<sub>6</sub>O

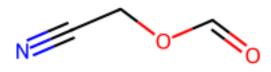
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.834 ± 4.689



SMILES: N#CCOC=O

Molecular Formula: C<sub>3</sub>H<sub>3</sub>NO<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.833 ± 4.970

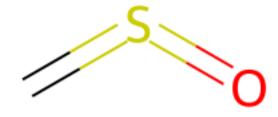


## **Molecule 113**

SMILES: C=S=O

Molecular Formula: CH<sub>2</sub>OS

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.829 ± 4.339

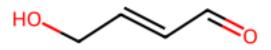


## **Molecule 114**

SMILES: O=CC=CCO

Molecular Formula: C<sub>4</sub>H<sub>6</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.828 ± 3.746



SMILES: OCS

Molecular Formula: CH4OS

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.824 ± 4.270

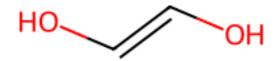


#### **Molecule 116**

SMILES: OC=CO

Molecular Formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.814 ± 4.089

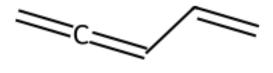


## **Molecule 117**

SMILES: C=C=CC=C

Molecular Formula: C<sub>5</sub>H<sub>6</sub>

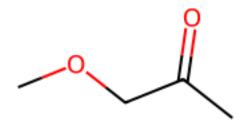
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.790 ± 4.575



SMILES: COCC(C)=O

Molecular Formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.781 ± 4.692

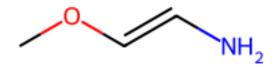


#### **Molecule 119**

SMILES: COC=CN

Molecular Formula: C<sub>3</sub>H<sub>7</sub>NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.765 ± 4.732

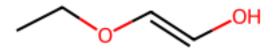


## **Molecule 120**

SMILES: CCOC=CO

Molecular Formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>

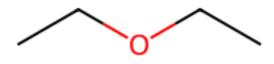
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.752 ± 4.800



SMILES: CCOCC

Molecular Formula: C<sub>4</sub>H<sub>10</sub>O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.738 ± 4.258

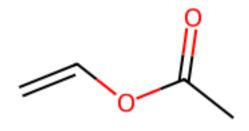


## **Molecule 122**

SMILES: C=COC(C)=O

Molecular Formula: C<sub>4</sub>H<sub>6</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.733 ± 4.719

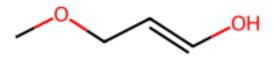


## **Molecule 123**

SMILES: COCC=CO

Molecular Formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>

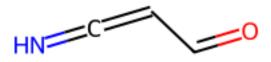
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.711 ± 4.621



SMILES: N=C=CC=O

Molecular Formula: C₃H₃NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.675 ± 3.944

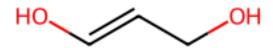


### **Molecule 125**

SMILES: OC=CCO

Molecular Formula: C<sub>3</sub>H<sub>6</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.673 ± 4.144

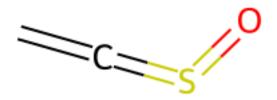


## **Molecule 126**

SMILES: C=C=S=O

Molecular Formula: C<sub>2</sub>H<sub>2</sub>OS

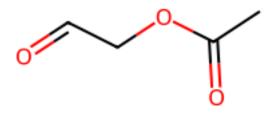
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.665 ± 4.576



SMILES: CC(=0)OCC=0

Molecular Formula: C<sub>4</sub>H<sub>6</sub>O<sub>3</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.663 ± 4.955

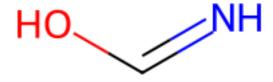


## **Molecule 128**

SMILES: N=CO

Molecular Formula: CH₃NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.607 ± 4.374

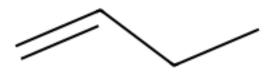


## **Molecule 129**

SMILES: C=CCC

Molecular Formula: C<sub>4</sub>H<sub>8</sub>

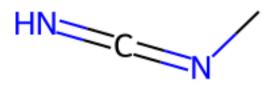
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.582 ± 3.193



SMILES: CN=C=N

Molecular Formula: C<sub>2</sub>H<sub>4</sub>N<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.573 ± 4.795



#### **Molecule 131**

SMILES: N=N

Molecular Formula: H<sub>2</sub>N<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.568 ± 4.570

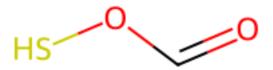


### **Molecule 132**

SMILES: O=COS

Molecular Formula: CH2O2S

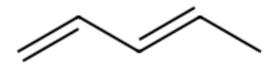
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.560 ± 4.990



SMILES: C=CC=CC

Molecular Formula: C₅H<sub>8</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.531 ± 3.688



## **Molecule 134**

SMILES: C=CCC=O

Molecular Formula: C<sub>4</sub>H<sub>6</sub>O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.523 ± 4.589



## **Molecule 135**

SMILES: NS

Molecular Formula: H₃NS

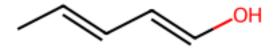
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.512 ± 3.235



SMILES: CC=CC=CO

Molecular Formula: C₅H<sub>8</sub>O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.505 ± 4.634

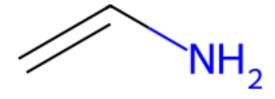


### **Molecule 137**

SMILES: C=CN

Molecular Formula: C<sub>2</sub>H<sub>5</sub>N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.502 ± 3.232

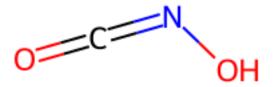


## **Molecule 138**

SMILES: O=C=NO

Molecular Formula: CHNO2

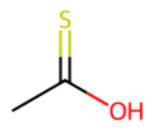
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.494 ± 3.839



SMILES: CC(O)=S

Molecular Formula: C<sub>2</sub>H<sub>4</sub>OS

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.458 ± 4.345



## **Molecule 140**

SMILES: COCC=S

Molecular Formula: C<sub>3</sub>H<sub>6</sub>OS

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.441 ± 4.828

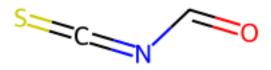


## Molecule 141

SMILES: O=CN=C=S

Molecular Formula: C₂HNOS

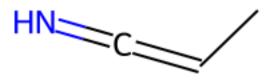
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.436 ± 4.825



SMILES: CC=C=N

Molecular Formula: C<sub>3</sub>H<sub>5</sub>N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.434 ± 4.789

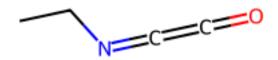


## **Molecule 143**

SMILES: CCN=C=C=O

Molecular Formula: C<sub>4</sub>H<sub>5</sub>NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.429 ± 4.686

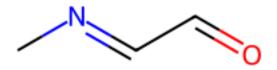


## **Molecule 144**

SMILES: CN=CC=O

Molecular Formula: C₃H₅NO

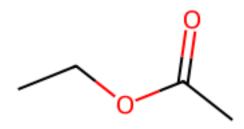
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.420 ± 4.514



SMILES: CCOC(C)=0

Molecular Formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.412 ± 4.230

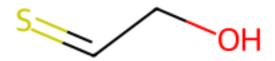


## **Molecule 146**

SMILES: OCC=S

Molecular Formula: C<sub>2</sub>H<sub>4</sub>OS

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.403 ± 4.269

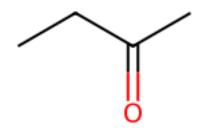


## **Molecule 147**

SMILES: CCC(C)=0

Molecular Formula: C<sub>4</sub>H<sub>8</sub>O

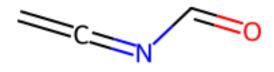
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.398 ± 4.243



SMILES: C=C=NC=O

Molecular Formula: C₃H₃NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.395 ± 4.900



## **Molecule 149**

SMILES: N=S

Molecular Formula: HNS

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.382 ± 3.384

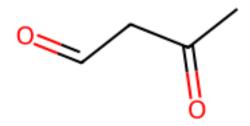


### **Molecule 150**

SMILES: CC(=0)CC=0

Molecular Formula: C<sub>4</sub>H<sub>6</sub>O<sub>2</sub>

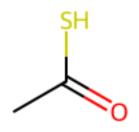
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.380 ± 4.809



SMILES: CC(=0)S

Molecular Formula: C<sub>2</sub>H<sub>4</sub>OS

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.347 ± 4.286

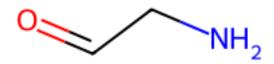


## **Molecule 152**

SMILES: NCC=O

Molecular Formula: C<sub>2</sub>H<sub>5</sub>NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.311 ± 4.350

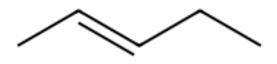


## **Molecule 153**

SMILES: CC=CCC

Molecular Formula: C<sub>5</sub>H<sub>10</sub>

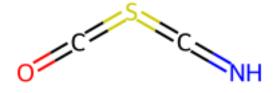
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.302 ± 4.823



SMILES: N=C=S=C=O

Molecular Formula: C₂HNOS

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.296 ± 4.874

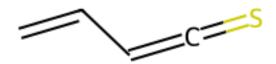


## **Molecule 155**

SMILES: C=CC=C=S

Molecular Formula: C<sub>4</sub>H<sub>4</sub>S

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.288 ± 4.573



## **Molecule 156**

SMILES: O=C=CC=S

Molecular Formula: C₃H₂OS

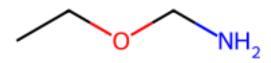
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.271 ± 4.855

0=C=-S

**SMILES: CCOCN** 

Molecular Formula: C₃H<sub>9</sub>NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.269 ± 4.958



## **Molecule 158**

SMILES: C=CC=CC=O

Molecular Formula: C₅H6O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.261 ± 3.967



## **Molecule 159**

SMILES: CC=S=O

Molecular Formula: C<sub>2</sub>H<sub>4</sub>OS

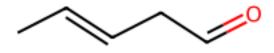
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.251 ± 4.770



SMILES: CC=CCC=O

Molecular Formula: C₅H<sub>8</sub>O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.243 ± 4.827

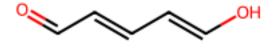


## **Molecule 161**

SMILES: O=CC=CC=CO

Molecular Formula: C<sub>5</sub>H<sub>6</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.235 ± 4.603

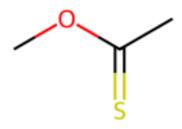


## **Molecule 162**

SMILES: COC(C)=S

Molecular Formula: C₃H<sub>6</sub>OS

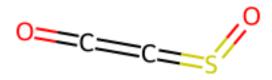
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.227 ± 4.798



SMILES: O=C=C=S=O

Molecular Formula: C<sub>2</sub>O<sub>2</sub>S

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.225 ± 4.974

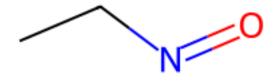


## **Molecule 164**

SMILES: CCN=O

Molecular Formula: C<sub>2</sub>H<sub>5</sub>NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.221 ± 4.877

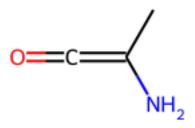


## **Molecule 165**

SMILES: CC(N)=C=O

Molecular Formula: C₃H₅NO

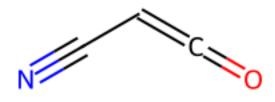
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.212 ± 4.286



SMILES: N#CC=C=O

Molecular Formula: C₃HNO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.200 ± 4.753



## **Molecule 167**

SMILES: O=CC=S

Molecular Formula: C<sub>2</sub>H<sub>2</sub>OS

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.198 ± 3.725



## **Molecule 168**

SMILES: O=S=CO

Molecular Formula: CH<sub>2</sub>O<sub>2</sub>S

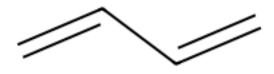
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.192 ± 4.424



SMILES: C=CC=C

Molecular Formula: C<sub>4</sub>H<sub>6</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.132 ± 3.563

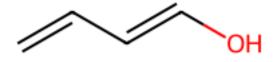


## **Molecule 170**

SMILES: C=CC=CO

Molecular Formula: C<sub>4</sub>H<sub>6</sub>O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.106 ± 3.408

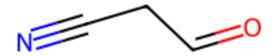


## **Molecule 171**

SMILES: N#CCC=O

Molecular Formula: C₃H₃NO

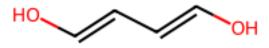
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.099 ± 3.896



SMILES: OC=CC=CO

Molecular Formula: C<sub>4</sub>H<sub>6</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.080 ± 4.693

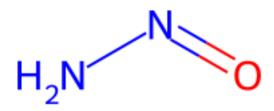


### **Molecule 173**

SMILES: NN=O

Molecular Formula: H<sub>2</sub>N<sub>2</sub>O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.072 ± 3.994

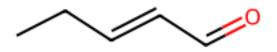


## **Molecule 174**

SMILES: CCC=CC=O

Molecular Formula: C₅H<sub>8</sub>O

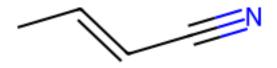
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.032 ± 4.228



SMILES: CC=CC#N

Molecular Formula: C<sub>4</sub>H<sub>5</sub>N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.996 ± 4.795

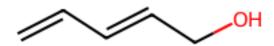


#### **Molecule 176**

SMILES: C=CC=CCO

Molecular Formula: C₅H<sub>8</sub>O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.965 ± 4.931

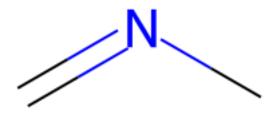


## **Molecule 177**

SMILES: C=NC

Molecular Formula: C<sub>2</sub>H<sub>5</sub>N

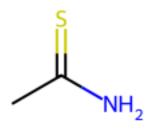
Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.956 ± 4.419



SMILES: CC(N)=S

Molecular Formula: C<sub>2</sub>H<sub>5</sub>NS

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.946 ± 4.526

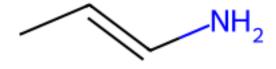


## **Molecule 179**

SMILES: CC=CN

Molecular Formula: C<sub>3</sub>H<sub>7</sub>N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.877 ± 4.585

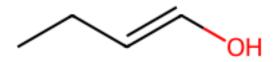


## Molecule 180

SMILES: CCC=CO

Molecular Formula: C<sub>4</sub>H<sub>8</sub>O

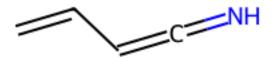
Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.877 ± 4.085



SMILES: C=CC=C=N

Molecular Formula: C<sub>4</sub>H<sub>5</sub>N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.812 ± 4.237

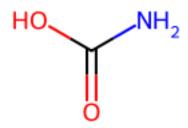


#### **Molecule 182**

SMILES: NC(=0)0

Molecular Formula: CH<sub>3</sub>NO<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.805 ± 4.982

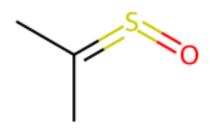


## Molecule 183

SMILES: CC(C)=S=O

Molecular Formula: C₃H<sub>6</sub>OS

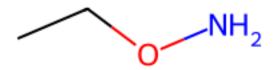
Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.801 ± 4.932



SMILES: CCON

Molecular Formula: C<sub>2</sub>H<sub>7</sub>NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.749 ± 4.659



#### **Molecule 185**

**SMILES: COCS** 

Molecular Formula: C<sub>2</sub>H<sub>6</sub>OS

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.749 ± 4.959

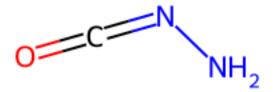


### **Molecule 186**

SMILES: NN=C=O

Molecular Formula: CH<sub>2</sub>N<sub>2</sub>O

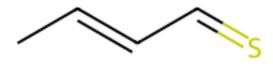
Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.736 ± 4.678



SMILES: CC=CC=S

Molecular Formula: C<sub>4</sub>H<sub>6</sub>S

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.734 ± 4.927

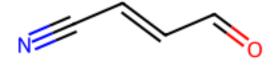


## **Molecule 188**

SMILES: N#CC=CC=O

Molecular Formula: C₄H₃NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.726 ± 4.749

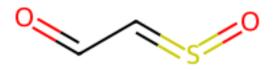


## Molecule 189

SMILES: O=CC=S=O

Molecular Formula: C<sub>2</sub>H<sub>2</sub>O<sub>2</sub>S

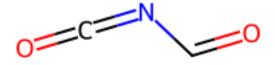
Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.688 ± 4.547



SMILES: O=C=NC=O

Molecular Formula: C<sub>2</sub>HNO<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.660 ± 4.417

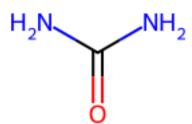


## **Molecule 191**

SMILES: NC(N)=O

Molecular Formula: CH<sub>4</sub>N<sub>2</sub>O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.633 ± 4.127

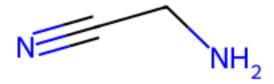


## **Molecule 192**

SMILES: N#CCN

Molecular Formula: C<sub>2</sub>H<sub>4</sub>N<sub>2</sub>

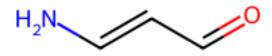
Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.627 ± 4.612



SMILES: NC=CC=O

Molecular Formula: C₃H₅NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.607 ± 3.170

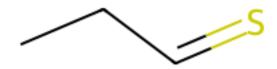


### **Molecule 194**

SMILES: CCC=S

Molecular Formula: C<sub>3</sub>H<sub>6</sub>S

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.607 ± 4.580

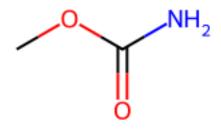


## **Molecule 195**

SMILES: COC(N)=O

Molecular Formula: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>

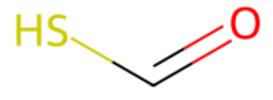
Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.601 ± 4.178



SMILES: O=CS

Molecular Formula: CH2OS

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.589 ± 4.291

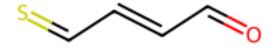


### **Molecule 197**

SMILES: O=CC=CC=S

Molecular Formula: C<sub>4</sub>H<sub>4</sub>OS

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.464 ± 4.713

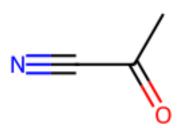


## Molecule 198

SMILES: CC(=0)C#N

Molecular Formula: C₃H₃NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.456 ± 4.414



SMILES: NC=CO

Molecular Formula: C<sub>2</sub>H<sub>5</sub>NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.452 ± 4.223

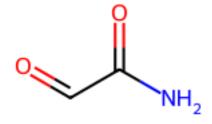


### **Molecule 200**

SMILES: NC(=0)C=0

Molecular Formula: C<sub>2</sub>H<sub>3</sub>NO<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.375 ± 4.769

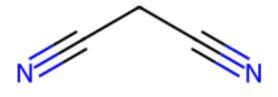


## **Molecule 201**

SMILES: N#CCC#N

Molecular Formula:  $C_3H_2N_2$ 

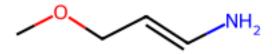
Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.353 ± 4.831



SMILES: COCC=CN

Molecular Formula: C<sub>4</sub>H<sub>9</sub>NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.349 ± 4.767

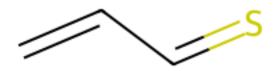


## **Molecule 203**

SMILES: C=CC=S

Molecular Formula: C<sub>3</sub>H<sub>4</sub>S

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.335 ± 3.958

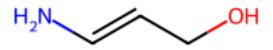


## **Molecule 204**

SMILES: NC=CCO

Molecular Formula: C<sub>3</sub>H<sub>7</sub>NO

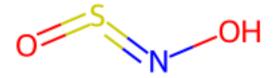
Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.311 ± 4.602



SMILES: O=S=NO

Molecular Formula: HNO<sub>2</sub>S

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.254 ± 4.576

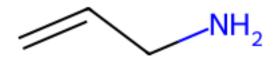


### **Molecule 206**

SMILES: C=CCN

Molecular Formula: C<sub>3</sub>H<sub>7</sub>N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.236 ± 4.827

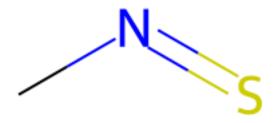


## **Molecule 207**

SMILES: CN=S

Molecular Formula: CH₃NS

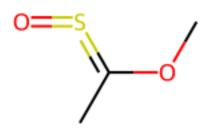
Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.229 ± 4.654



SMILES: COC(C)=S=O

Molecular Formula: C<sub>3</sub>H<sub>6</sub>O<sub>2</sub>S

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.178 ± 4.720



## **Molecule 209**

SMILES: N#CC=S

Molecular Formula: C2HNS

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.175 ± 4.580



## **Molecule 210**

SMILES: C=CC=CCC

Molecular Formula: C<sub>6</sub>H<sub>10</sub>

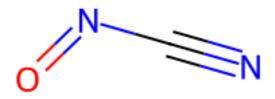
Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.169 ± 4.791



SMILES: N#CN=O

Molecular Formula: CN2O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.057 ± 4.235

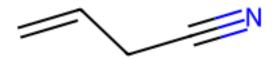


## **Molecule 212**

SMILES: C=CCC#N

Molecular Formula: C<sub>4</sub>H<sub>5</sub>N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.023 ± 4.787

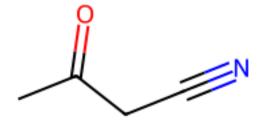


## **Molecule 213**

SMILES: CC(=0)CC#N

Molecular Formula: C₄H₅NO

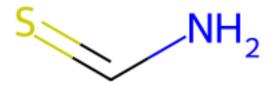
Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.966 ± 4.833



SMILES: NC=S

Molecular Formula: CH₃NS

Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.961 ± 3.551



#### **Molecule 215**

SMILES: CON=S=O

Molecular Formula: CH₃NO₂S

Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.937 ± 4.863

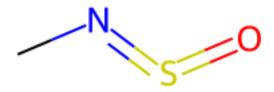


## **Molecule 216**

SMILES: CN=S=O

Molecular Formula: CH₃NOS

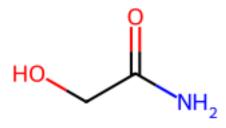
Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.913 ± 4.609



SMILES: NC(=0)CO

Molecular Formula: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.873 ± 4.875



## **Molecule 218**

SMILES: C=CC=S=O

Molecular Formula: C₃H₄OS

Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.826 ± 4.914



## **Molecule 219**

SMILES: NC=S=O

Molecular Formula: CH₃NOS

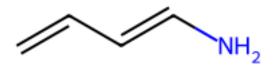
Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.809 ± 3.858



SMILES: C=CC=CN

Molecular Formula: C<sub>4</sub>H<sub>7</sub>N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.744 ± 4.278

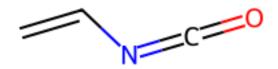


## **Molecule 221**

SMILES: C=CN=C=O

Molecular Formula: C₃H₃NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.716 ± 4.721

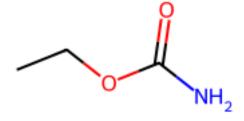


## **Molecule 222**

SMILES: CCOC(N)=O

Molecular Formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>

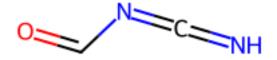
Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.685 ± 4.934



SMILES: N=C=NC=O

Molecular Formula: C<sub>2</sub>H<sub>2</sub>N<sub>2</sub>O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.672 ± 4.974

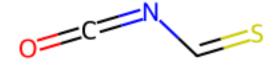


### **Molecule 224**

SMILES: O=C=NC=S

Molecular Formula: C2HNOS

Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.649 ± 4.936



### **Molecule 225**

SMILES: N#CC=S=O

Molecular Formula: C₂HNOS

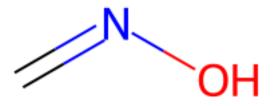
Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.641 ± 4.516

N 5 0

SMILES: C=NO

Molecular Formula: CH₃NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.630 ± 4.847

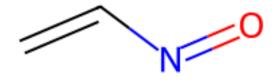


### **Molecule 227**

SMILES: C=CN=O

Molecular Formula: C<sub>2</sub>H<sub>3</sub>NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.607 ± 4.647

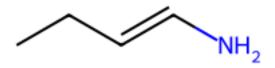


## **Molecule 228**

SMILES: CCC=CN

Molecular Formula: C<sub>4</sub>H<sub>9</sub>N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.515 ± 4.526



SMILES: CC(N)=S=O

Molecular Formula: C<sub>2</sub>H<sub>5</sub>NOS

Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.509 ± 4.856

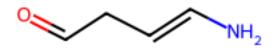


## **Molecule 230**

SMILES: NC=CCC=O

Molecular Formula: C<sub>4</sub>H<sub>7</sub>NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.456 ± 4.509

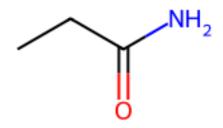


## **Molecule 231**

SMILES: CCC(N)=O

Molecular Formula: C<sub>3</sub>H<sub>7</sub>NO

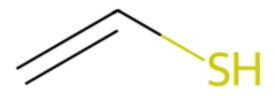
Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.433 ± 4.425



SMILES: C=CS

Molecular Formula: C<sub>2</sub>H<sub>4</sub>S

Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.373 ± 4.083

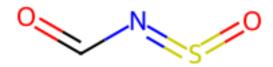


#### **Molecule 233**

SMILES: O=CN=S=O

Molecular Formula: CHNO<sub>2</sub>S

Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.341 ± 4.990

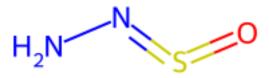


# **Molecule 234**

SMILES: NN=S=O

 $Molecular\ Formula:\ H_2N_2OS$ 

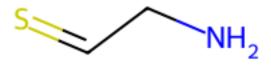
Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.314 ± 4.974



SMILES: NCC=S

Molecular Formula: C<sub>2</sub>H<sub>5</sub>NS

Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.260 ± 4.874

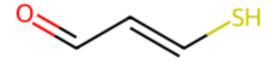


## **Molecule 236**

SMILES: O=CC=CS

Molecular Formula: C<sub>3</sub>H<sub>4</sub>OS

Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.215 ± 4.685

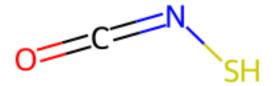


## **Molecule 237**

SMILES: O=C=NS

Molecular Formula: CHNOS

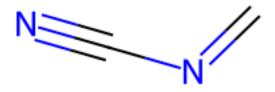
Predicted Column Density ( $log_{10} cm^{-2}$ ): 11.997 ± 4.372



SMILES: C=NC#N

Molecular Formula: C<sub>2</sub>H<sub>2</sub>N<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 11.935 ± 4.937

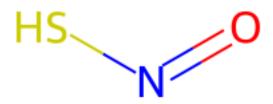


### **Molecule 239**

SMILES: O=NS

Molecular Formula: HNOS

Predicted Column Density ( $log_{10} cm^{-2}$ ): 11.683 ± 4.505

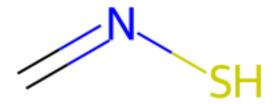


### **Molecule 240**

SMILES: C=NS

Molecular Formula: CH₃NS

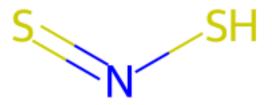
Predicted Column Density ( $log_{10} cm^{-2}$ ): 11.194 ± 4.177



SMILES: S=NS

Molecular Formula: HNS2

Predicted Column Density ( $log_{10} cm^{-2}$ ): 10.512 ± 4.919



## **Molecule 242**

SMILES: O=S=NS

Molecular Formula: HNOS2

Predicted Column Density ( $log_{10} cm^{-2}$ ): 10.467 ± 4.635

