Molecule 1

SMILES: OO

Molecular Formula: H_2O_2

Predicted Column Density ($\log_{10}$ cm^{-2}): 18.485 ± 2.437
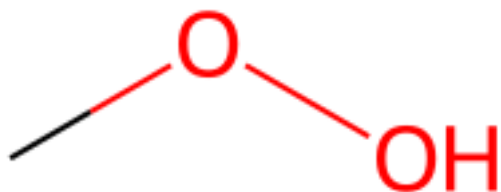

Molecule 2

SMILES: COO

Molecular Formula: CH_4O_2

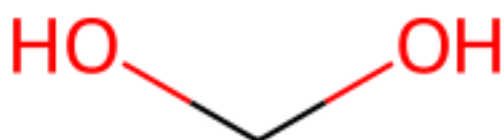Predicted Column Density ($\log_{10}$ cm^{-2}): 18.165 ± 3.271

Molecule 3

SMILES: OCO

Molecular Formula: CH_4O_2

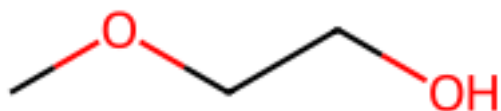Predicted Column Density ($\log_{10}$ cm^{-2}): 18.068 ± 2.266

Molecule 4

SMILES: COCCO

Molecular Formula: $C_3H_8O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 17.359 ± 3.739

Molecule 5

SMILES: CC

Molecular Formula: C_2H_6

Predicted Column Density ($\log_{10}$ cm^{-2}): 17.325 ± 2.276

Molecule 6

SMILES: COCOO

Molecular Formula: $C_2H_6O_3$

Predicted Column Density ($\log_{10}$ cm^{-2}): 17.267 ± 3.957
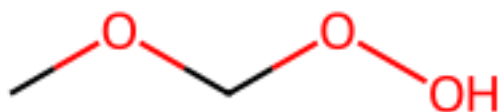
Molecule 7

SMILES: S=C=S

Molecular Formula: CS_2

Predicted Column Density ($\log_{10}$ cm^{-2}): 17.267 ± 3.699
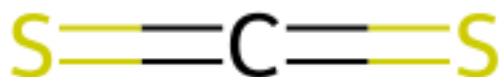
Molecule 8

SMILES: O=CCCO

Molecular Formula: $C_3H_6O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 17.186 ± 3.773
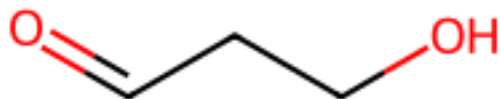
Molecule 9

SMILES: COC=C=O

Molecular Formula: $C_3H_4O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 17.111 ± 2.854
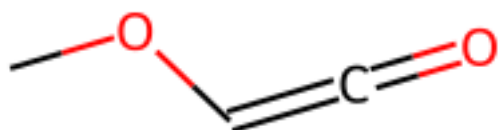
Molecule 10

SMILES: O=CCOO

Molecular Formula: $C_2H_4O_3$

Predicted Column Density ($\log_{10}$ cm^{-2}): 17.043 ± 3.964
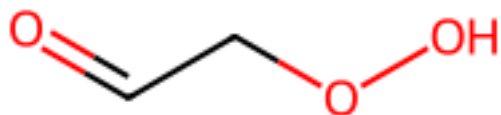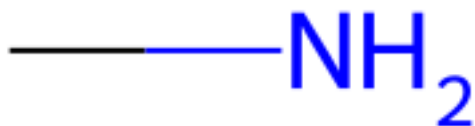

Molecule 11

SMILES: CN

Molecular Formula: CH_5N

Predicted Column Density ($\log_{10}$ cm^{-2}): 17.043 ± 1.391

Molecule 12

SMILES: C=COC

Molecular Formula: C_3H_6O

Predicted Column Density ($\log_{10}$ cm^{-2}): 17.009 ± 2.325
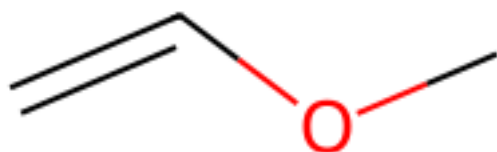
Molecule 13

SMILES: O=C=O

Molecular Formula: CO_2

Predicted Column Density ($\log_{10}$ cm^{-2}): 16.989 ± 2.656

O===C===O

Molecule 14

SMILES: COCOC

Molecular Formula: $C_3H_8O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 16.802 ± 3.067

Molecule 15

SMILES: CC=COC

Molecular Formula: C_4H_8O

Predicted Column Density ($\log_{10}$ cm^{-2}): 16.796 ± 3.407
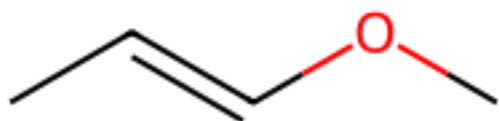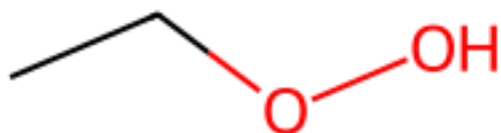
Molecule 16

SMILES: CCOO

Molecular Formula: $C_2H_6O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 16.778 ± 3.912
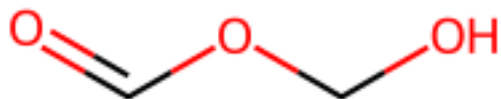

Molecule 17

SMILES: O=COCO

Molecular Formula: $C_2H_4O_3$

Predicted Column Density ($\log_{10}$ cm^{-2}): 16.774 ± 2.974
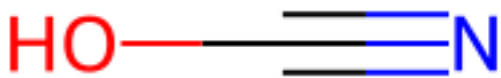

Molecule 18

SMILES: N#CO

Molecular Formula: CHNO

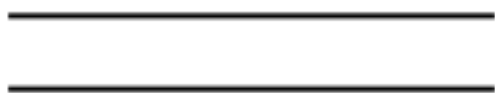Predicted Column Density ($\log_{10}$ cm^{-2}): 16.665 ± 3.192

Molecule 19

SMILES: C=C

Molecular Formula: C_2H_4

Predicted Column Density (log_{10} cm^{-2}): 16.586 ± 1.805

Molecule 20

SMILES: CN=C=S

Molecular Formula: C_2H_3NS

Predicted Column Density (log_{10} cm^{-2}): 16.584 ± 3.080
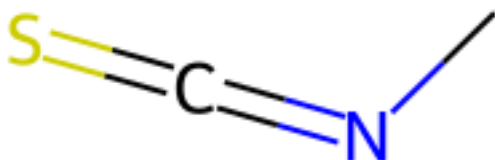
Molecule 21

SMILES: COCC=O

Molecular Formula: $C_3H_6O_2$

Predicted Column Density (log_{10} cm^{-2}): 16.578 ± 3.031
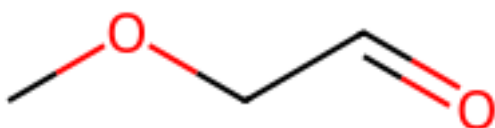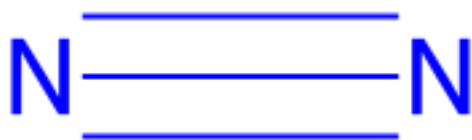
Molecule 22

SMILES: N#N

Molecular Formula: N_2

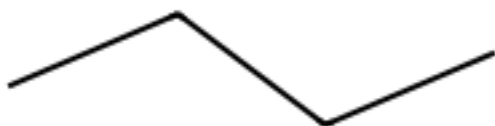Predicted Column Density ($\log_{10}$ cm^{-2}): 16.549 ± 2.333

Molecule 23

SMILES: CCCC

Molecular Formula: C_4H_{10}

Predicted Column Density ($\log_{10}$ cm^{-2}): 16.488 ± 3.536
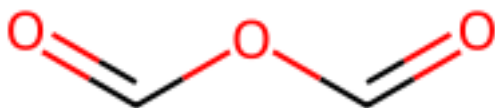

Molecule 24

SMILES: O=COC=O

Molecular Formula: $C_2H_2O_3$

Predicted Column Density ($\log_{10}$ cm^{-2}): 16.486 ± 3.884

Molecule 25

SMILES: CCCOC

Molecular Formula: $C_4H_{10}O$

Predicted Column Density ($\log_{10}$ cm^{-2}): 16.484 ± 3.655
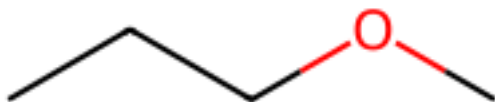
Molecule 26

SMILES: COC=CO

Molecular Formula: $C_3H_6O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 16.472 ± 3.140
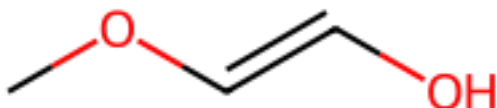
Molecule 27

SMILES: C=COCO

Molecular Formula: $C_3H_6O_2$

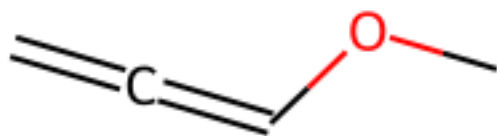Predicted Column Density ($\log_{10}$ cm^{-2}): 16.415 ± 3.566
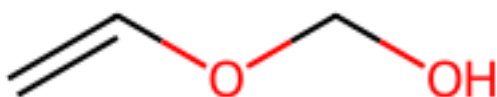
Molecule 28

SMILES: C=C=COC

Molecular Formula: C_4H_6O

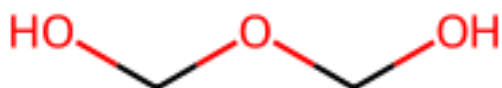Predicted Column Density ($\log_{10}$ cm^{-2}): 16.385 ± 3.963

Molecule 29

SMILES: OCOCO

Molecular Formula: $C_2H_6O_3$

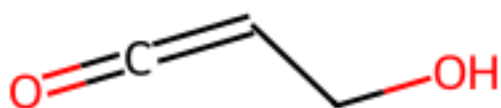Predicted Column Density ($\log_{10}$ cm^{-2}): 16.384 ± 3.096

Molecule 30

SMILES: O=C=CCO

Molecular Formula: $C_3H_4O_2$

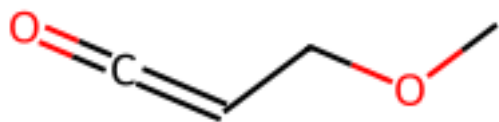Predicted Column Density ($\log_{10}$ cm^{-2}): 16.381 ± 2.742

Molecule 31

SMILES: COCC=C=O

Molecular Formula: $C_4H_6O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 16.340 ± 3.977
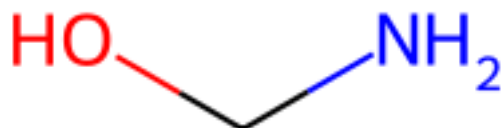
Molecule 32

SMILES: NCO

Molecular Formula: CH_5NO

Predicted Column Density ($\log_{10}$ cm^{-2}): 16.328 ± 3.161

Molecule 33

SMILES: COC=CC=O

Molecular Formula: $C_4H_6O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 16.317 ± 2.798

Molecule 34

SMILES: CCCC=O

Molecular Formula: C_4H_8O

Predicted Column Density ($\log_{10}$ cm^{-2}): 16.310 ± 3.898

Molecule 35

SMILES: C#C

Molecular Formula: C_2H_2

Predicted Column Density ($\log_{10}$ cm^{-2}): 16.235 ± 3.751
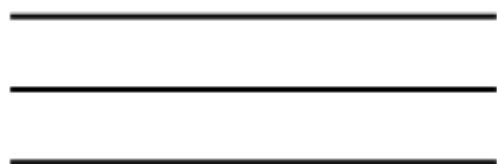
Molecule 36

SMILES: CC=COCO

Molecular Formula: $C_4H_8O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 16.202 ± 3.932
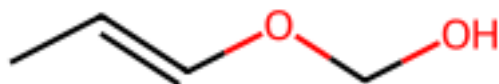
Molecule 37

SMILES: O=C=C=O

Molecular Formula: C_2O_2

Predicted Column Density ($\log_{10}$ cm^{-2}): 16.137 ± 3.769
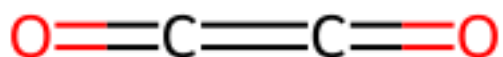
Molecule 38

SMILES: C=C=NC

Molecular Formula: C_3H_5N

Predicted Column Density ($\log_{10}$ cm^{-2}): 16.076 ± 3.176
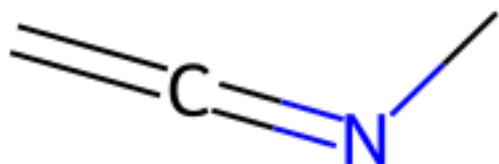
Molecule 39

SMILES: O=C=NCO

Molecular Formula: $C_2H_3NO_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 16.062 ± 2.957
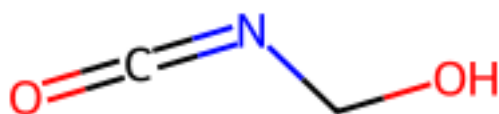
Molecule 40

SMILES: CCN

Molecular Formula: C_2H_7N

Predicted Column Density ($\log_{10}$ cm^{-2}): 16.027 ± 2.876
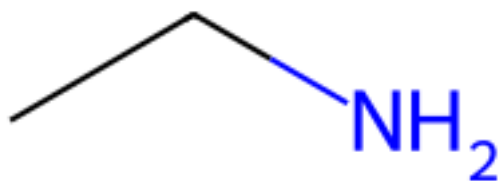
Molecule 41

SMILES: O=C=C=S

Molecular Formula: C_2OS

Predicted Column Density ($\log_{10}$ cm^{-2}): 16.017 ± 2.617
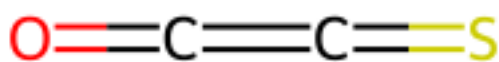
Molecule 42

SMILES: CCOC=O

Molecular Formula: $C_3H_6O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.991 ± 2.981
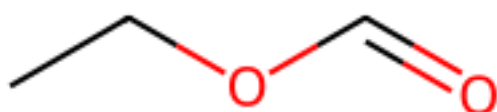
Molecule 43

SMILES: COC#N

Molecular Formula: C_2H_3NO

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.952 ± 3.146

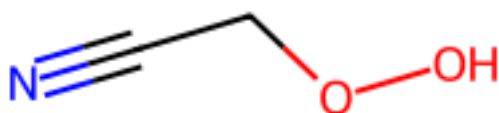## Molecule 44

SMILES: N#CCOO

Molecular Formula: $C_2H_3NO_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.939 ± 3.836

Molecule 45

SMILES: S=C=C=S

Molecular Formula: C_2S_2

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.898 ± 3.915

Molecule 46

SMILES: OS

Molecular Formula: H_2OS

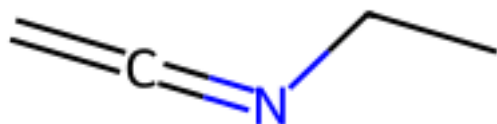Predicted Column Density ($\log_{10}$ cm^{-2}): 15.815 ± 2.067

Molecule 47

SMILES: C=C=NCC

Molecular Formula: C_4H_7N

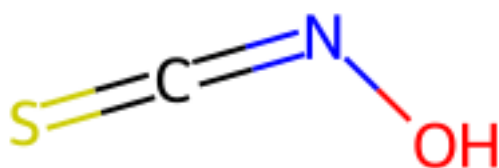Predicted Column Density ($\log_{10}$ cm^{-2}): 15.790 ± 3.796

Molecule 48

SMILES: ON=C=S

Molecular Formula: CHNOS

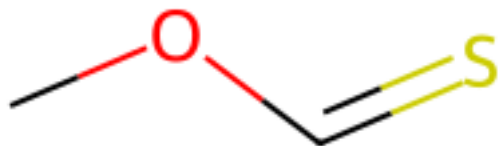Predicted Column Density ($\log_{10}$ cm^{-2}): 15.790 ± 3.775

Molecule 49

SMILES: COC=S

Molecular Formula: C_2H_4OS

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.785 ± 3.225

Molecule 50

SMILES: C1COCO1

Molecular Formula: $C_3H_6O_2$

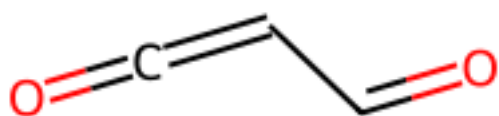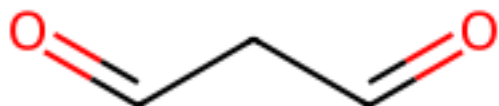Predicted Column Density ($\log_{10}$ cm^{-2}): 15.763 ± 3.601

Molecule 51

SMILES: O=C=CC=O

Molecular Formula: $C_3H_2O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.759 ± 2.555

Molecule 52

SMILES: C=C=C

Molecular Formula: C_3H_4

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.751 ± 2.779

Molecule 53

SMILES: O=CCC=O

Molecular Formula: $C_3H_4O_2$

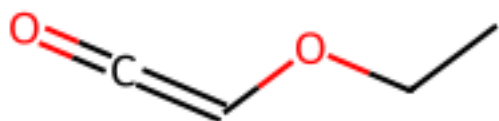Predicted Column Density ($\log_{10}$ cm^{-2}): 15.738 ± 3.649

Molecule 54

SMILES: CCOC=C=O

Molecular Formula: $C_4H_6O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.735 ± 3.578

Molecule 55

SMILES: CCC=C=O

Molecular Formula: C_4H_6O

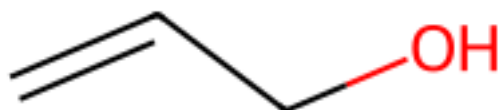Predicted Column Density ($\log_{10}$ cm^{-2}): 15.660 ± 3.218
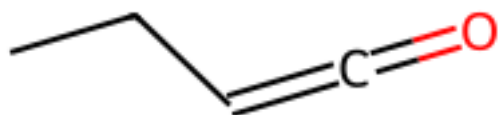
Molecule 56

SMILES: C=CCO

Molecular Formula: C_3H_6O

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.645 ± 2.376
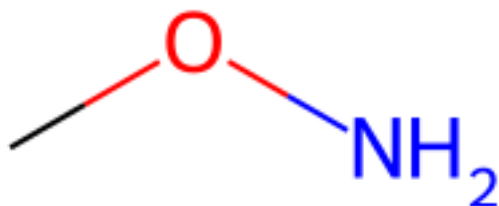
Molecule 57

SMILES: CON

Molecular Formula: CH_5NO

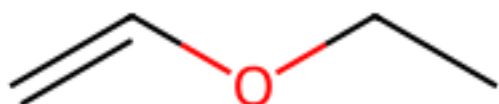Predicted Column Density ($\log_{10}$ cm^{-2}): 15.644 ± 3.557

Molecule 58

SMILES: C=COCC

Molecular Formula: C_4H_8O

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.632 ± 3.423

Molecule 59

SMILES: O=CC=O

Molecular Formula: $C_2H_2O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.611 ± 2.206

Molecule 60

SMILES: CC(C)=C=O

Molecular Formula: C_4H_6O

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.605 ± 3.623
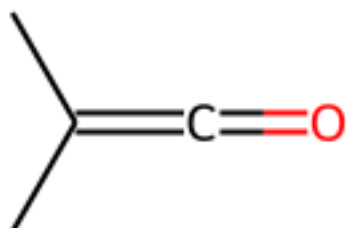
Molecule 61

SMILES: C=CCOC

Molecular Formula: C_4H_8O
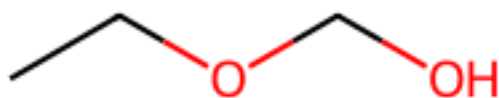
Predicted Column Density ($\log_{10}$ cm^{-2}): 15.603 ± 3.665
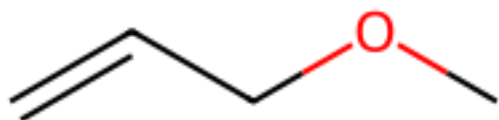
Molecule 62

SMILES: CCOCO

Molecular Formula: $C_3H_8O_2$

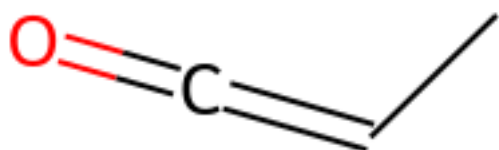Predicted Column Density ($\log_{10}$ cm^{-2}): 15.601 ± 2.731

Molecule 63

SMILES: CC=C=O

Molecular Formula: C_3H_4O

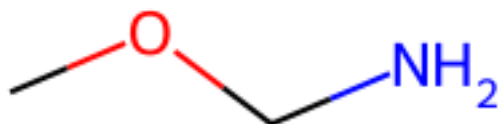Predicted Column Density ($\log_{10}$ cm^{-2}): 15.596 ± 2.982

Molecule 64

SMILES: COCN

Molecular Formula: C_2H_7NO

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.593 ± 3.494

Molecule 65

SMILES: C=CC=COC

Molecular Formula: C_5H_8O

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.571 ± 3.826
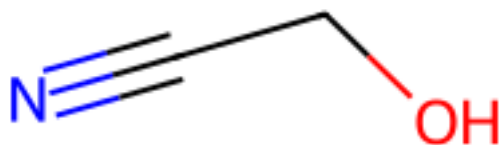

Molecule 66

SMILES: C=C=N

Molecular Formula: C_2H_3N

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.554 ± 3.010
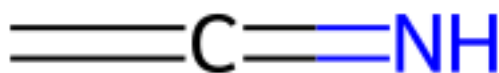
Molecule 67

SMILES: N#CCO

Molecular Formula: C_2H_3NO

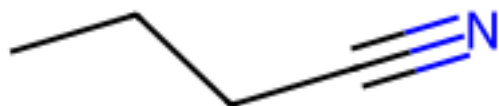Predicted Column Density ($\log_{10}$ cm^{-2}): 15.535 ± 2.073

Molecule 68

SMILES: CCCC#N

Molecular Formula: C_4H_7N

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.501 ± 3.901

Molecule 69

SMILES: NN

Molecular Formula: H_4N_2

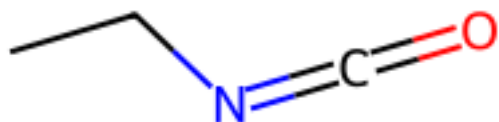Predicted Column Density ($\log_{10}$ cm^{-2}): 15.492 ± 2.292

Molecule 70

SMILES: CCN=C=O

Molecular Formula: C_3H_5NO

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.477 ± 2.883

Molecule 71

SMILES: COCC#N

Molecular Formula: C_3H_5NO

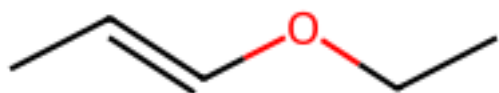Predicted Column Density ($\log_{10}$ cm^{-2}): 15.474 ± 2.850
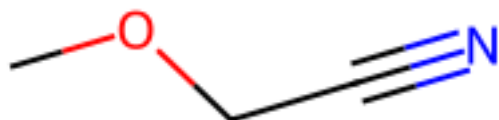
Molecule 72

SMILES: CC=COCC

Molecular Formula: $C_5H_{10}O$

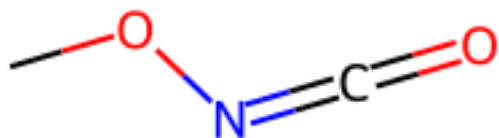Predicted Column Density ($\log_{10}$ cm^{-2}): 15.419 ± 3.960

Molecule 73

SMILES: CON=C=O

Molecular Formula: $C_2H_3NO_2$

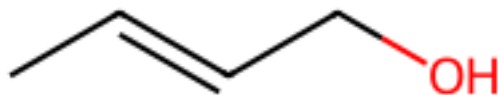Predicted Column Density ($\log_{10}$ cm^{-2}): 15.392 ± 3.755

Molecule 74

SMILES: CC=CCO

Molecular Formula: C_4H_8O

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.391 ± 3.305
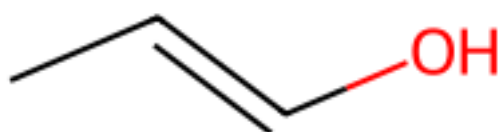

Molecule 75

SMILES: CC=CO

Molecular Formula: C_3H_6O

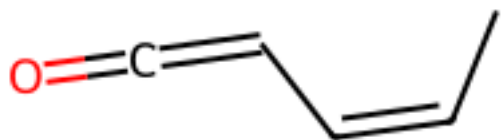Predicted Column Density ($\log_{10}$ cm^{-2}): 15.376 ± 3.245

Molecule 76

SMILES: C/C=C\C=C=O

Molecular Formula: C_5H_6O

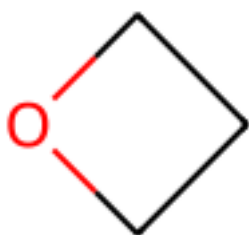Predicted Column Density ($\log_{10}$ cm^{-2}): 15.368 ± 3.619

Molecule 77

SMILES: C1COC1

Molecular Formula: C_3H_6O

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.357 ± 2.510

Molecule 78

SMILES: CC=CCOC

Molecular Formula: $C_5H_{10}O$

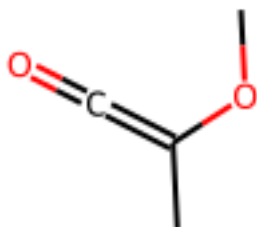Predicted Column Density ($\log_{10}$ cm^{-2}): 15.349 ± 3.792

Molecule 79

SMILES: COC(C)=C=O

Molecular Formula: $C_4H_6O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.331 ± 3.250

Molecule 80

SMILES: COC=S=O

Molecular Formula: $C_2H_4O_2S$

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.317 ± 3.757

Molecule 81

SMILES: N#CC=O

Molecular Formula: C_2HNO

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.303 ± 2.725

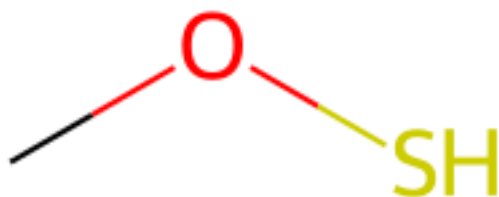## Molecule 82

SMILES: C#[SH]

Molecular Formula: CH_2S

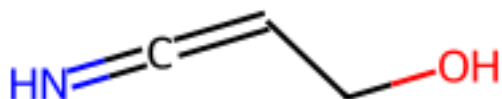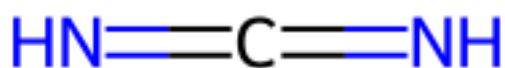Predicted Column Density ($\log_{10}$ cm^{-2}): 15.284 ± 2.396

Molecule 83

SMILES: C=C=NO

Molecular Formula: C_2H_3NO

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.281 ± 3.873
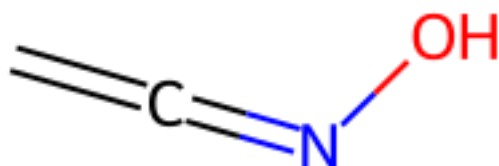
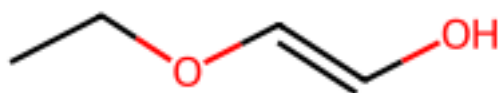## Molecule 84

SMILES: NCOC=O

Molecular Formula: $C_2H_5NO_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.271 ± 3.962
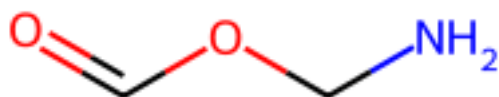
Molecule 85

SMILES: CC=CC=O

Molecular Formula: C_4H_6O

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.221 ± 2.357
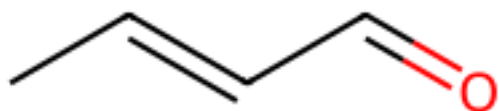
Molecule 86

SMILES: COS

Molecular Formula: CH_4OS

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.205 ± 2.987

Molecule 87

SMILES: COC(C)=O

Molecular Formula: $C_3H_6O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.170 ± 2.332
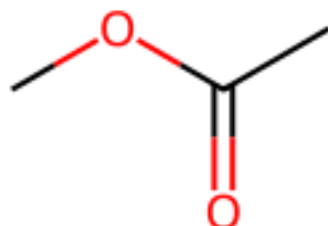
Molecule 88

SMILES: N=C=CCO

Molecular Formula: C_3H_5NO

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.112 ± 3.811

Molecule 89

SMILES: N=C=N

Molecular Formula: CH_2N_2

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.103 ± 3.720

Molecule 90

SMILES: CCOC=CO

Molecular Formula: $C_4H_8O_2$

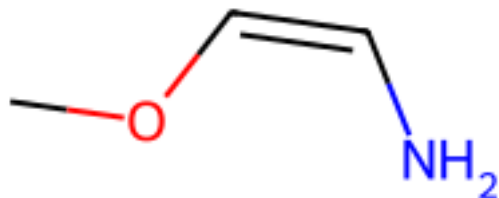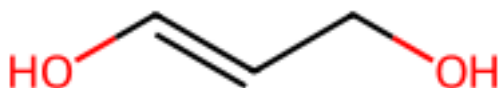Predicted Column Density ($\log_{10}$ cm^{-2}): 15.095 ± 3.564

Molecule 91

SMILES: CO/C=C\N

Molecular Formula: C_3H_7NO

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.093 ± 3.699

Molecule 92

SMILES: O/C=C/CO

Molecular Formula: $C_3H_6O_2$

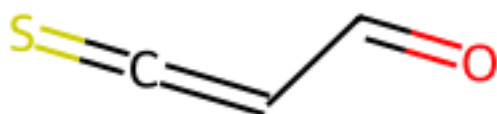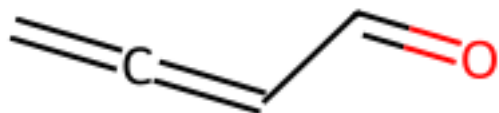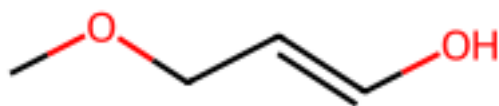Predicted Column Density ($\log_{10}$ cm^{-2}): 15.067 ± 3.187

Molecule 93

SMILES: O=CC=C=S

Molecular Formula: C_3H_2OS

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.064 ± 3.107

Molecule 94

SMILES: OC=CO

Molecular Formula: $C_2H_4O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.052 ± 3.152

Molecule 95

SMILES: C=C=CC=O

Molecular Formula: C_4H_4O

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.032 ± 2.961

Molecule 96

SMILES: COCC=CO

Molecular Formula: $C_4H_8O_2$

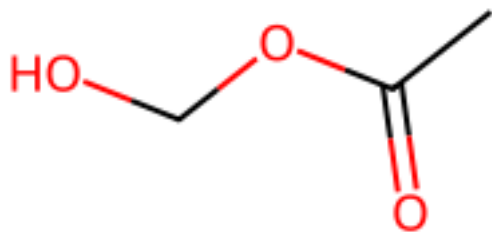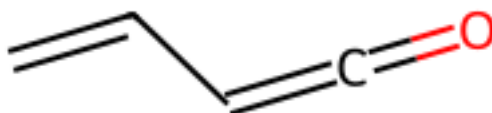Predicted Column Density ($\log_{10}$ cm^{-2}): 15.026 ± 3.634

Molecule 97

SMILES: CC(=O)OCO

Molecular Formula: $C_3H_6O_3$

Predicted Column Density ($\log_{10}$ cm^{-2}): 15.015 ± 3.359

Molecule 98

SMILES: C=CC=C=O

Molecular Formula: C_4H_4O

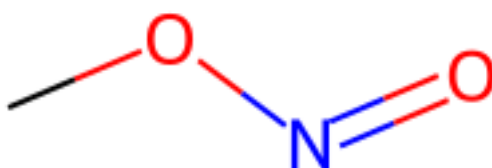Predicted Column Density ($\log_{10}$ cm^{-2}): 15.013 ± 2.602

Molecule 99

SMILES: CON=O

Molecular Formula: CH_3NO_2

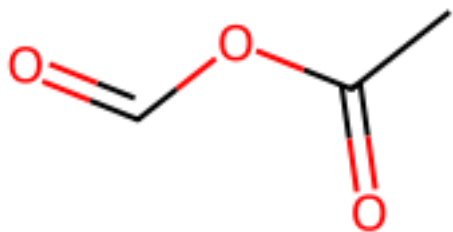Predicted Column Density ($\log_{10}$ cm^{-2}): 14.992 ± 2.731

Molecule 100

SMILES: CC(=O)OC=O

Molecular Formula: $C_3H_4O_3$

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.977 ± 3.620

Molecule 101

SMILES: O=C=NO

Molecular Formula: $CHNO_2$

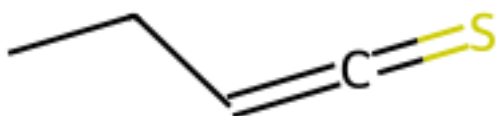Predicted Column Density ($\log_{10}$ cm^{-2}): 14.967 ± 2.966
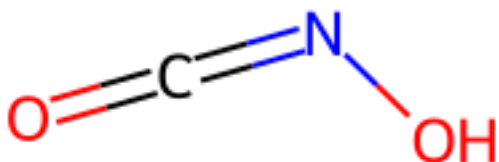
Molecule 102

SMILES: CCC=C=S

Molecular Formula: C_4H_6S

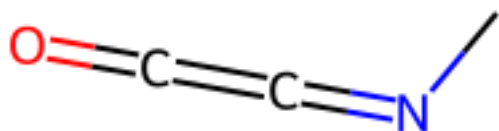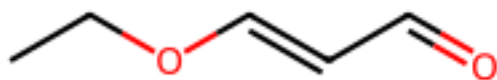Predicted Column Density ($\log_{10}$ cm^{-2}): 14.966 ± 3.870

Molecule 103

SMILES: CN=C=C=O

Molecular Formula: C_3H_3NO

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.948 ± 3.295

Molecule 104

SMILES: CCOC=CC=O

Molecular Formula: $C_5H_8O_2$

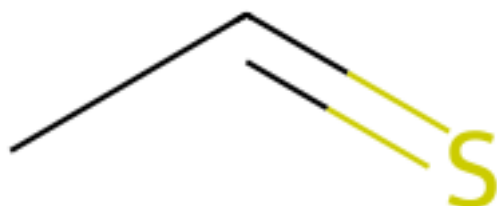Predicted Column Density ($\log_{10}$ cm^{-2}): 14.940 ± 3.747

Molecule 105

SMILES: CC=S

Molecular Formula: C_2H_4S

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.937 ± 2.948

Molecule 106

SMILES: OCS

Molecular Formula: CH_4OS

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.933 ± 3.276

Molecule 107

SMILES: C=CCC

Molecular Formula: C_4H_8

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.924 ± 2.410
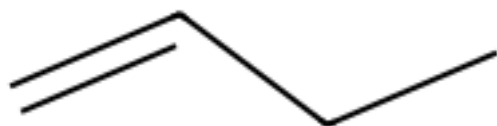
Molecule 108

SMILES: O=C/C=C\CO

Molecular Formula: $C_4H_6O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.912 ± 2.813
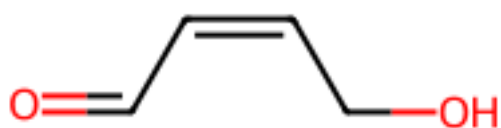
Molecule 109

SMILES: CC=C=S

Molecular Formula: C_3H_4S

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.902 ± 3.705
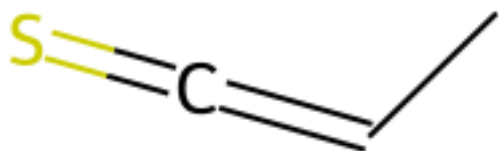
Molecule 110

SMILES: CC(C)=S

Molecular Formula: C_3H_6S

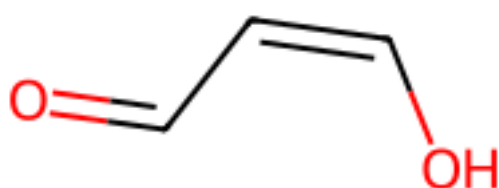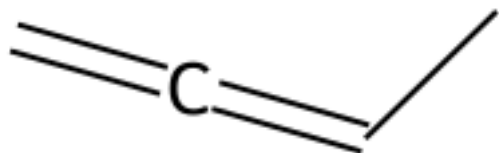Predicted Column Density ($\log_{10}$ cm^{-2}): 14.901 ± 3.253
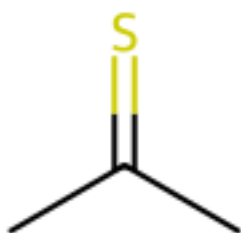
Molecule 111

SMILES: O=C/C=C\O

Molecular Formula: $C_3H_4O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.897 ± 1.245

Molecule 112

SMILES: C=C=CC

Molecular Formula: C_4H_6

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.870 ± 3.953

Molecule 113

SMILES: O=S=C=S

Molecular Formula: COS_2

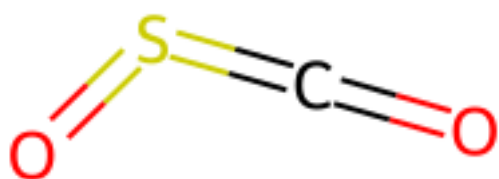Predicted Column Density ($\log_{10}$ cm^{-2}): 14.868 ± 3.191
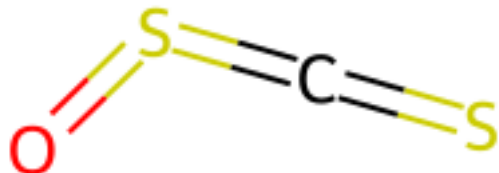
Molecule 114

SMILES: O=C=S=O

Molecular Formula: CO_2S

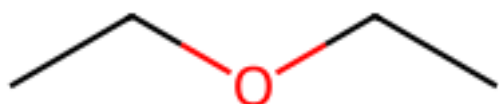Predicted Column Density ($\log_{10}$ cm^{-2}): 14.820 ± 3.351

Molecule 115

SMILES: CCOCC

Molecular Formula: $C_4H_{10}O$

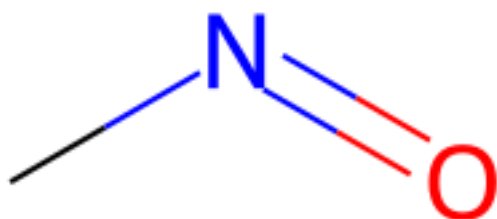Predicted Column Density ($\log_{10}$ cm^{-2}): 14.818 ± 3.127

Molecule 116

SMILES: CN=O

Molecular Formula: CH_3NO

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.797 ± 2.992
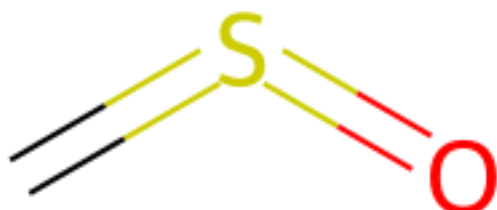
Molecule 117

SMILES: C=S=O

Molecular Formula: CH_2OS

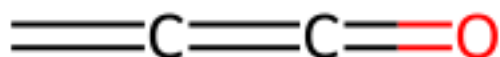Predicted Column Density ($\log_{10}$ cm^{-2}): 14.793 ± 3.564

Molecule 118

SMILES: C=C=C=O

Molecular Formula: C_3H_2O

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.768 ± 3.100

Molecule 119

SMILES: C=CCC=O

Molecular Formula: C_4H_6O
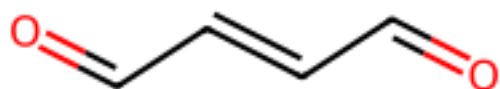
Predicted Column Density ($\log_{10}$ cm^{-2}): 14.763 ± 3.906

Molecule 120

SMILES: O=CC=CC=O

Molecular Formula: $C_4H_4O_2$

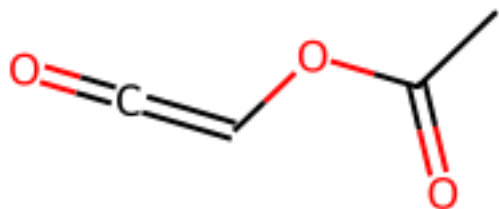Predicted Column Density ($\log_{10}$ cm^{-2}): 14.742 ± 2.925

Molecule 121

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

Molecular Formula: $C_4H_4O_3$

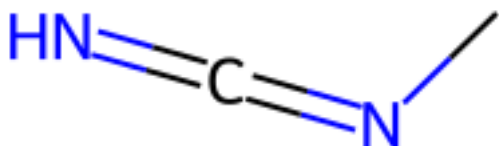Predicted Column Density ($\log_{10}$ cm^{-2}): 14.721 ± 3.711

Molecule 122

SMILES: CN=C=N

Molecular Formula: $C_2H_4N_2$

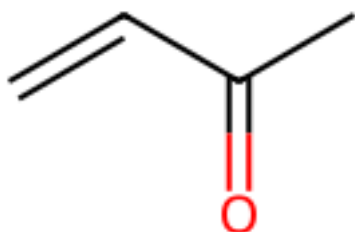Predicted Column Density ($\log_{10}$ cm^{-2}): 14.713 ± 3.743

Molecule 123

SMILES: C=CC(C)=O

Molecular Formula: C_4H_6O

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.709 ± 3.763

Molecule 124

SMILES: N=C=C=O

Molecular Formula: C_2HNO

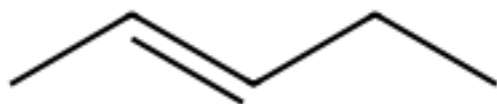Predicted Column Density ($\log_{10}$ cm^{-2}): 14.707 ± 3.127

Molecule 125

SMILES: CC=CCC

Molecular Formula: C_5H_{10}

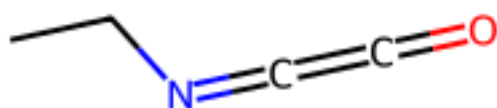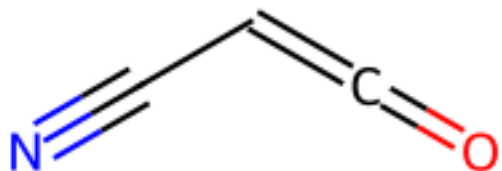Predicted Column Density ($\log_{10}$ cm^{-2}): 14.670 ± 3.797

Molecule 126

SMILES: CCN=C=C=O

Molecular Formula: C_4H_5NO

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.663 ± 3.591

Molecule 127

SMILES: C=C=C=S

Molecular Formula: C_3H_2S

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.649 ± 3.667

Molecule 128

SMILES: N#CC=C=O

Molecular Formula: C_3HNO

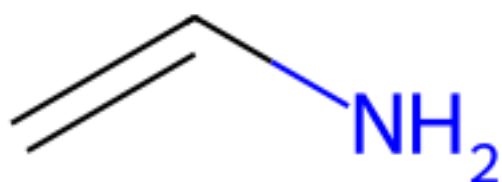Predicted Column Density ($\log_{10}$ cm^{-2}): 14.645 ± 3.908

Molecule 129

SMILES: C=CN

Molecular Formula: C_2H_5N

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.640 ± 2.463

Molecule 130

SMILES: OCC=S

Molecular Formula: C_2H_4OS

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.631 ± 3.504
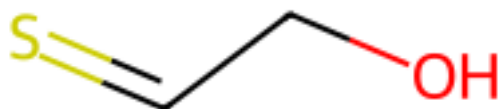
Molecule 131

SMILES: N#CCC=O

Molecular Formula: C_3H_3NO

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.625 ± 3.133
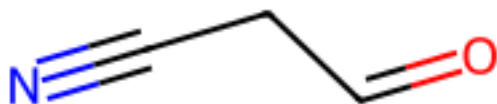
Molecule 132

SMILES: C=COC(C)=O

Molecular Formula: $C_4H_6O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.618 ± 3.748
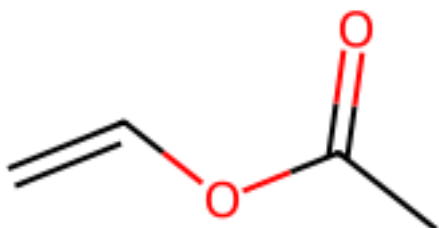
Molecule 133

SMILES: NS

Molecular Formula: H_3NS

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.600 ± 2.408

Molecule 134

SMILES: COCC=S

Molecular Formula: C_3H_6OS

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.589 ± 3.989
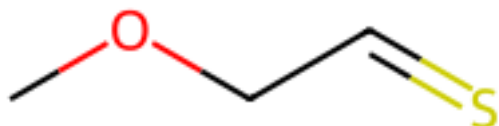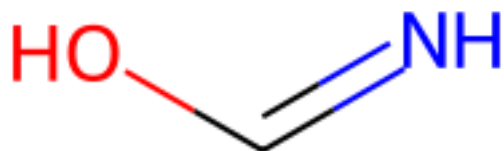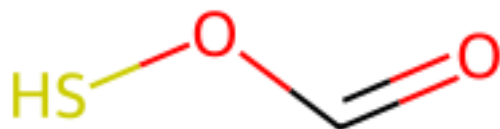

Molecule 135

SMILES: NCC=O

Molecular Formula: C_2H_5NO

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.582 ± 3.427
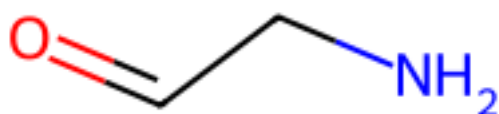
Molecule 136

SMILES: N=CO

Molecular Formula: CH_3NO

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.572 ± 3.630

Molecule 137

SMILES: O=COS

Molecular Formula: CH_2O_2S

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.547 ± 3.886
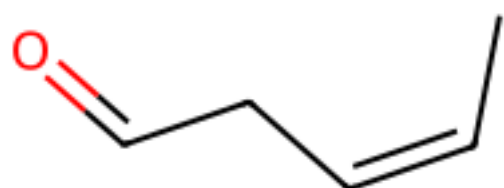

Molecule 138

SMILES: C/C=C\CC=O

Molecular Formula: C_5H_8O

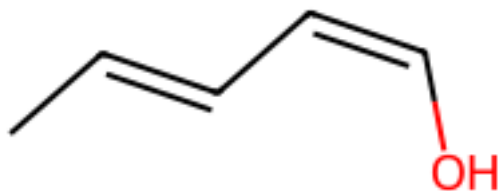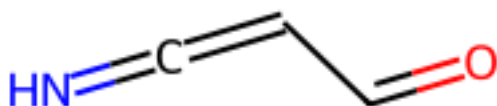Predicted Column Density ($\log_{10}$ cm^{-2}): 14.509 ± 3.903

Molecule 139

SMILES: C/C=C/C=C\O

Molecular Formula: C_5H_8O

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.507 ± 3.334

Molecule 140

SMILES: N=C=CC=O

Molecular Formula: C_3H_3NO

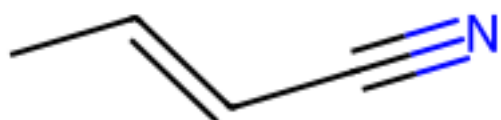Predicted Column Density ($\log_{10}$ cm^{-2}): 14.490 ± 3.027

Molecule 141

SMILES: CC=CC#N

Molecular Formula: C_4H_5N

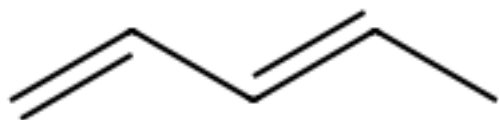Predicted Column Density ($\log_{10}$ cm^{-2}): 14.488 ± 3.769

Molecule 142

SMILES: C=CC=CC

Molecular Formula: C_5H_8

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.476 ± 2.773

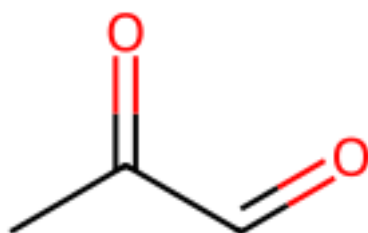## Molecule 143

SMILES: CC(=O)C=O

Molecular Formula: $C_3H_4O_2$

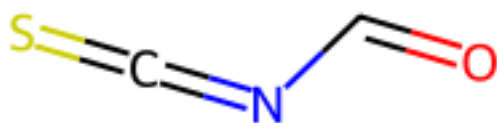Predicted Column Density ($\log_{10}$ cm^{-2}): 14.470 ± 3.581

Molecule 144

SMILES: O=CN=C=S

Molecular Formula: C_2HNOS

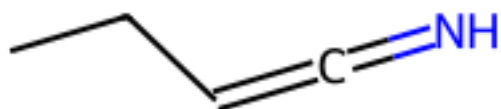Predicted Column Density ($\log_{10}$ cm^{-2}): 14.455 ± 3.968

Molecule 145

SMILES: CCC=C=N

Molecular Formula: C_4H_7N

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.391 ± 3.821

Molecule 146

SMILES: C=C=S=O

Molecular Formula: C_2H_2OS

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.390 ± 3.647
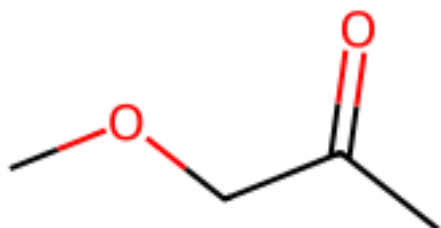
Molecule 147

SMILES: COCC(C)=O

Molecular Formula: $C_4H_8O_2$

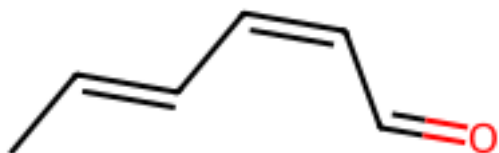Predicted Column Density ($\log_{10}$ cm^{-2}): 14.382 ± 3.936

Molecule 148

SMILES: C/C=C/C=C\C=O

Molecular Formula: C_6H_8O

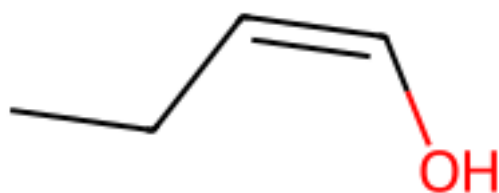Predicted Column Density ($\log_{10}$ cm^{-2}): 14.352 ± 3.783

Molecule 149

SMILES: CC/C=C\O

Molecular Formula: C_4H_8O

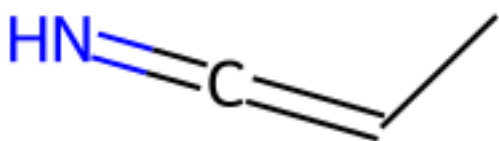Predicted Column Density ($\log_{10}$ cm^{-2}): 14.346 ± 3.100

Molecule 150

SMILES: CC=C=N

Molecular Formula: C_3H_5N

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.328 ± 3.811

Molecule 151

SMILES: N=N

Molecular Formula: H_2N_2

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.324 ± 3.896

Molecule 152

SMILES: C=CC=C=S

Molecular Formula: C_4H_4S

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.319 ± 3.710
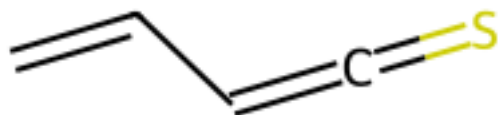
Molecule 153

SMILES: O=S=CO

Molecular Formula: CH_2O_2S

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.316 ± 3.634
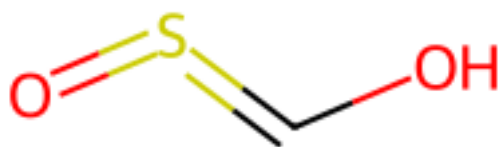
Molecule 154

SMILES: CC=S=O

Molecular Formula: C_2H_4OS

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.294 ± 3.936

Molecule 155

SMILES: CC(O)=S

Molecular Formula: C_2H_4OS

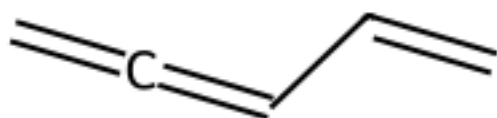Predicted Column Density ($\log_{10}$ cm^{-2}): 14.293 ± 3.450
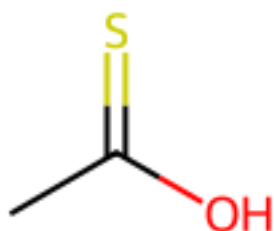
Molecule 156

SMILES: C=C=CC=C

Molecular Formula: C_5H_6

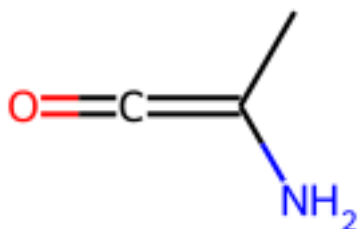Predicted Column Density ($\log_{10}$ cm^{-2}): 14.287 ± 3.607

Molecule 157

SMILES: CC(N)=C=O

Molecular Formula: C_3H_5NO

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.261 ± 3.378

Molecule 158

SMILES: N=S

Molecular Formula: HNS

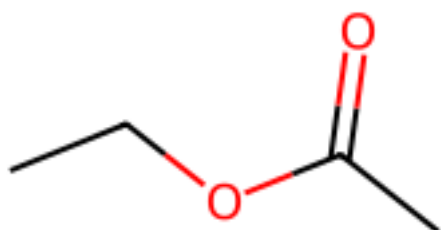Predicted Column Density ($\log_{10}$ cm^{-2}): 14.243 ± 2.723

Molecule 159

SMILES: CCOC(C)=O

Molecular Formula: $C_4H_8O_2$

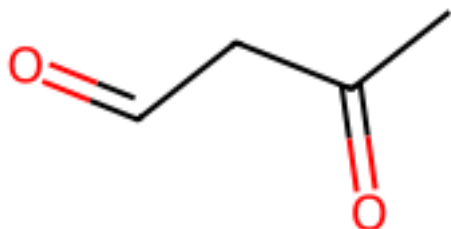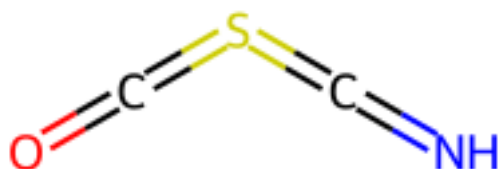Predicted Column Density ($\log_{10}$ cm^{-2}): 14.232 ± 3.280

Molecule 160

SMILES: CC(=O)CC=O

Molecular Formula: $C_4H_6O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.225 ± 3.927

Molecule 161

SMILES: N=C=S=C=O

Molecular Formula: C_2HNOS

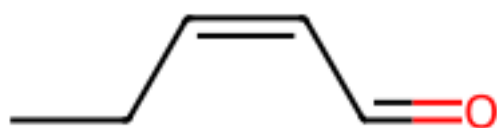Predicted Column Density ($\log_{10}$ cm^{-2}): 14.194 ± 3.983

Molecule 162

SMILES: CC/C=C\C=O

Molecular Formula: C_5H_8O

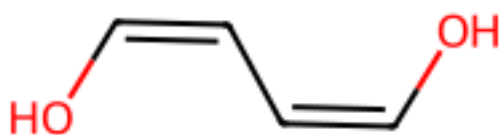Predicted Column Density ($\log_{10}$ cm^{-2}): 14.191 ± 3.137

Molecule 163

SMILES: O/C=C\C=C/O

Molecular Formula: $C_4H_6O_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.183 ± 3.309

Molecule 164

SMILES: CN=CC=O

Molecular Formula: C_3H_5NO

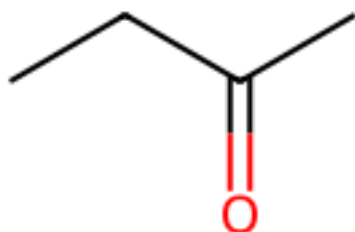Predicted Column Density ($\log_{10}$ cm^{-2}): 14.168 ± 3.430
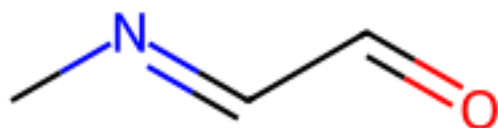
Molecule 165

SMILES: CCC(C)=O

Molecular Formula: C_4H_8O

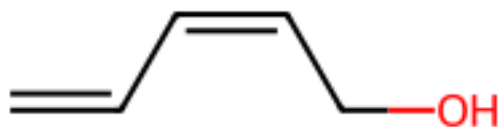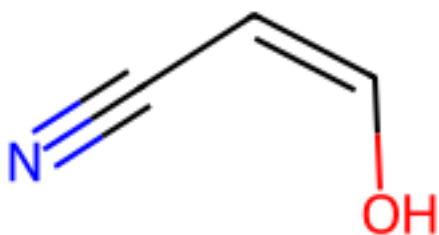Predicted Column Density ($\log_{10}$ cm^{-2}): 14.168 ± 3.294

Molecule 166

SMILES: C=C/C=C\CO

Molecular Formula: C_5H_8O

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.166 ± 3.952

Molecule 167

SMILES: N#C/C=C\O

Molecular Formula: C_3H_3NO

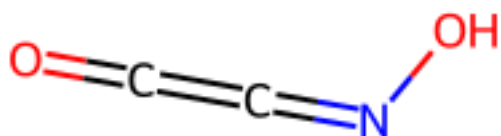Predicted Column Density ($\log_{10}$ cm^{-2}): 14.164 ± 3.994

Molecule 168

SMILES: O=C=C=NO

Molecular Formula: C_2HNO_2

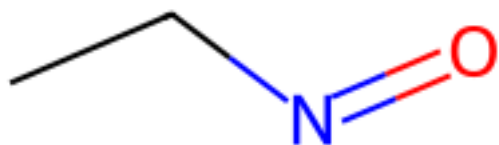Predicted Column Density ($\log_{10}$ cm^{-2}): 14.153 ± 3.961

Molecule 169

SMILES: CCN=O

Molecular Formula: C_2H_5NO

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.153 ± 3.919

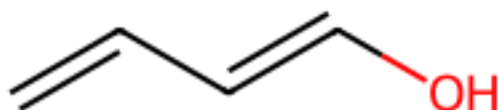## Molecule 170

SMILES: C=CC=CO

Molecular Formula: C_4H_6O

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.152 ± 2.497

Molecule 171

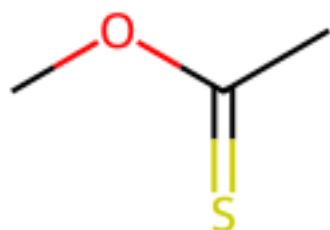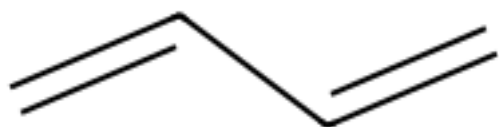SMILES: COC(C)=S

Molecular Formula: C_3H_6OS

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.149 ± 3.805

Molecule 172

SMILES: C=CC=C

Molecular Formula: C_4H_6

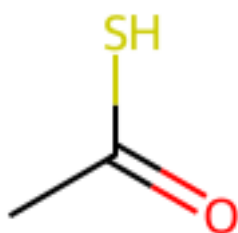Predicted Column Density ($\log_{10}$ cm^{-2}): 14.120 ± 2.652

Molecule 173

SMILES: CC(=O)S

Molecular Formula: C_2H_4OS

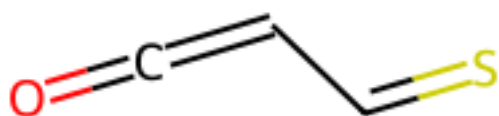Predicted Column Density ($\log_{10}$ cm^{-2}): 14.107 ± 3.126

Molecule 174

SMILES: O=C=CC=S

Molecular Formula: C_3H_2OS

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.100 ± 3.984

Molecule 175

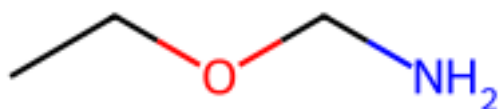SMILES: CCOCN

Molecular Formula: C_3H_9NO

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.098 ± 3.914

Molecule 176

SMILES: NC(=O)O

Molecular Formula: CH_3NO_2

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.087 ± 3.968
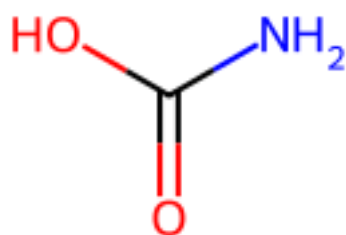
Molecule 177

SMILES: CC(=O)OC=CO

Molecular Formula: $C_4H_6O_3$

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.082 ± 3.976
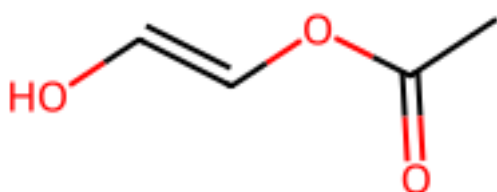
Molecule 178

SMILES: NCN=C=O

Molecular Formula: $C_2H_4N_2O$

Predicted Column Density ($\log_{10}$ cm^{-2}): 14.079 ± 3.962
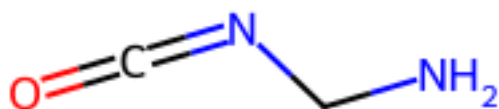
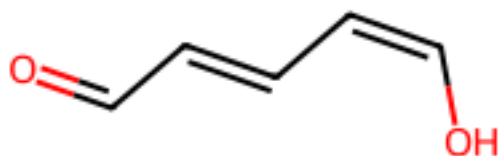## Molecule 179

SMILES: O=CC=C/C=C\O

Molecular Formula: $C_5H_6O_2$
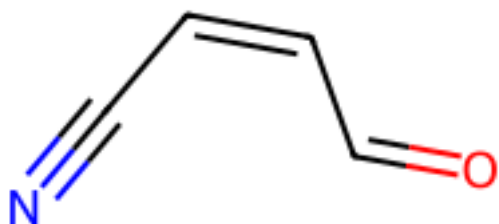
Predicted Column Density ($\log_{10}$ cm^{-2}): 14.028 ± 3.275

Molecule 180

SMILES: N#C/C=C\C=O

Molecular Formula: C_4H_3NO

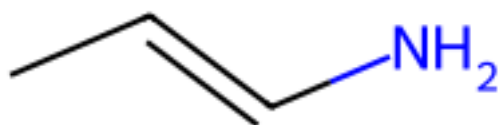Predicted Column Density ($\log_{10}$ cm^{-2}): 14.009 ± 3.816

Molecule 181

SMILES: C/C=C/N

Molecular Formula: C_3H_7N

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.997 ± 3.742

Molecule 182

SMILES: C=CC=CC=O

Molecular Formula: C_5H_6O

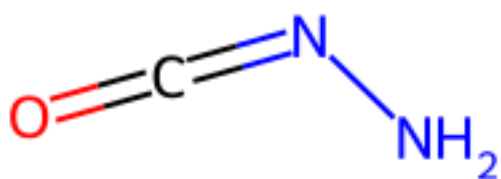Predicted Column Density ($\log_{10}$ cm^{-2}): 13.997 ± 3.007

Molecule 183

SMILES: NN=C=O

Molecular Formula: CH_2N_2O

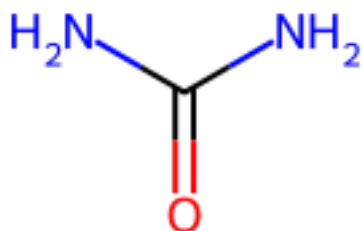Predicted Column Density ($\log_{10}$ cm^{-2}): 13.992 ± 3.785

Molecule 184

SMILES: NC(N)=O

Molecular Formula: CH_4N_2O

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.976 ± 2.960

Molecule 185

SMILES: O=CC=S

Molecular Formula: C_2H_2OS
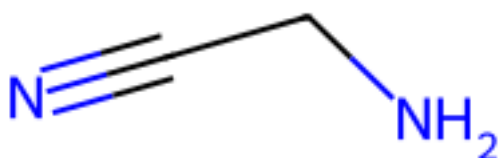
Predicted Column Density ($\log_{10}$ cm^{-2}): 13.953 ± 2.905

Molecule 186

SMILES: N#CCN

Molecular Formula: $C_2H_4N_2$
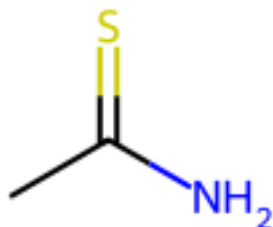
Predicted Column Density ($\log_{10}$ cm^{-2}): 13.924 ± 3.558

Molecule 187

SMILES: CC(N)=S

Molecular Formula: C_2H_5NS

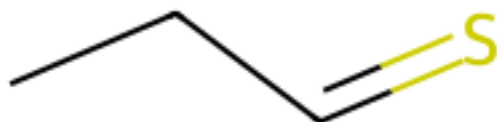Predicted Column Density ($\log_{10}$ cm^{-2}): 13.911 ± 3.649

Molecule 188

SMILES: CCC=S

Molecular Formula: C_3H_6S

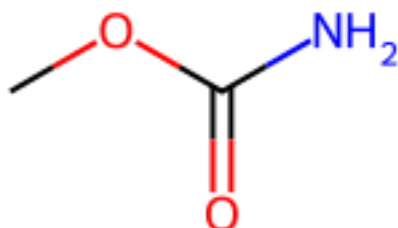Predicted Column Density ($\log_{10}$ cm^{-2}): 13.910 ± 3.665

Molecule 189

SMILES: COC(N)=O

Molecular Formula: $C_2H_5NO_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.904 ± 3.251

Molecule 190

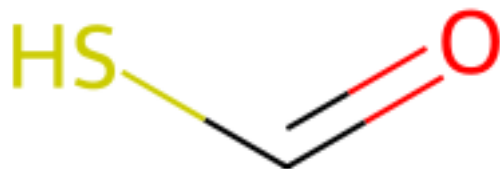SMILES: O=CS

Molecular Formula: CH_2OS

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.893 ± 3.224

Molecule 191

SMILES: N#CCC#N

Molecular Formula: $C_3H_2N_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.875 ± 3.797
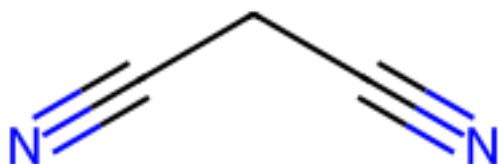
Molecule 192

SMILES: COCS

Molecular Formula: C_2H_6OS

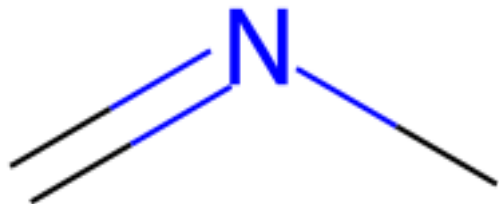Predicted Column Density ($\log_{10}$ cm^{-2}): 13.861 ± 3.786
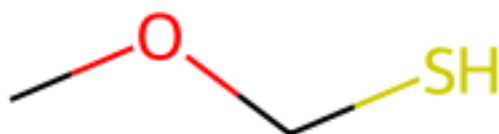
Molecule 193

SMILES: C=NC

Molecular Formula: C_2H_5N

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.847 ± 3.371
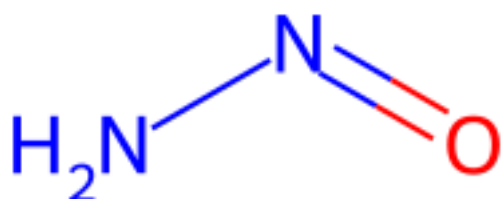

Molecule 194

SMILES: NN=O

Molecular Formula: H_2N_2O

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.820 ± 3.187
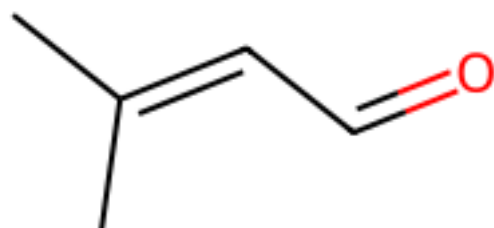

Molecule 195

SMILES: CC(C)=CC=O

Molecular Formula: C_5H_8O

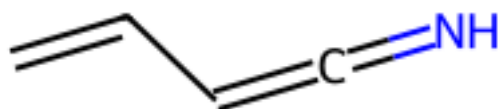Predicted Column Density ($\log_{10}$ cm^{-2}): 13.818 ± 3.918

Molecule 196

SMILES: C=CC=C=N

Molecular Formula: C_4H_5N

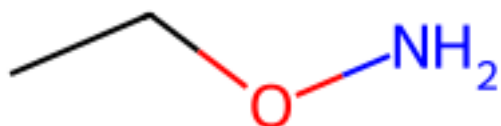Predicted Column Density ($\log_{10}$ cm^{-2}): 13.745 ± 3.314

Molecule 197

SMILES: CCON

Molecular Formula: C_2H_7NO

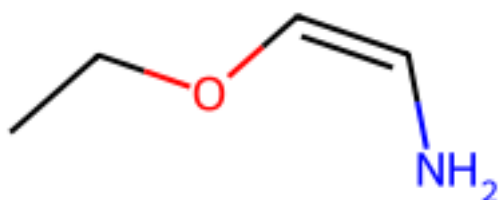Predicted Column Density ($\log_{10}$ cm^{-2}): 13.718 ± 3.785

Molecule 198

SMILES: CCO/C=C\N

Molecular Formula: C_4H_9NO

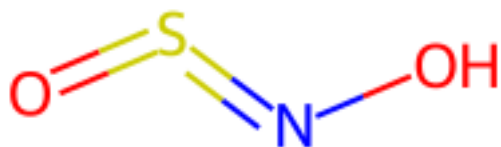Predicted Column Density ($\log_{10}$ cm^{-2}): 13.716 ± 3.893

Molecule 199

SMILES: O=S=NO

Molecular Formula: HNO_2S

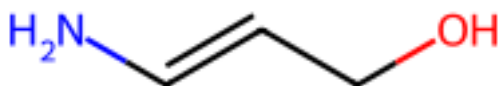Predicted Column Density ($\log_{10}$ cm^{-2}): 13.696 ± 3.747

Molecule 200

SMILES: NC=CCO

Molecular Formula: C_3H_7NO

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.688 ± 3.611

Molecule 201

SMILES: NC=CO

Molecular Formula: C_2H_5NO

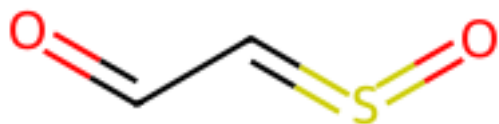Predicted Column Density ($\log_{10}$ cm^{-2}): 13.674 ± 3.360

Molecule 202

SMILES: O=CC=S=O

Molecular Formula: $C_2H_2O_2S$

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.654 ± 3.702
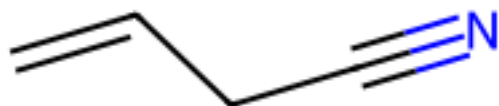
Molecule 203

SMILES: C=CCC#N

Molecular Formula: C_4H_5N

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.650 ± 3.910
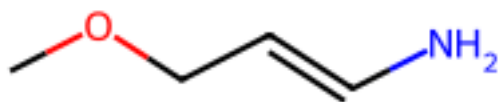
Molecule 204

SMILES: COCC=CN

Molecular Formula: C_4H_9NO

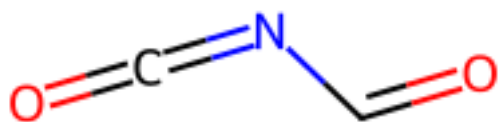Predicted Column Density ($\log_{10}$ cm^{-2}): 13.647 ± 3.713

Molecule 205

SMILES: O=C=NC=O

Molecular Formula: C_2HNO_2

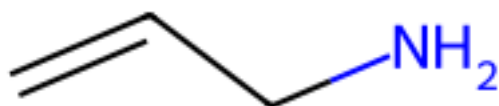Predicted Column Density ($\log_{10}$ cm^{-2}): 13.633 ± 3.540

Molecule 206

SMILES: C=CCN

Molecular Formula: C_3H_7N

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.607 ± 3.830

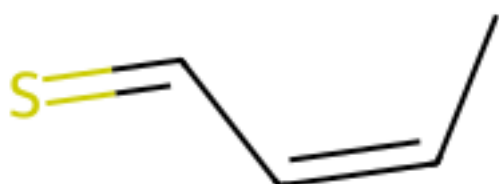## Molecule 207

SMILES: C/C=C\C=S

Molecular Formula: C_4H_6S

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.563 ± 3.880

Molecule 208

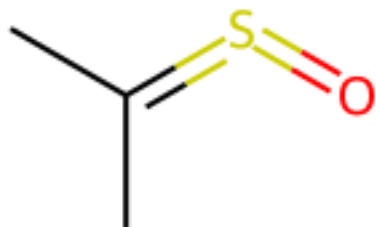SMILES: CC(C)=S=O

Molecular Formula: C_3H_6OS

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.537 ± 3.863

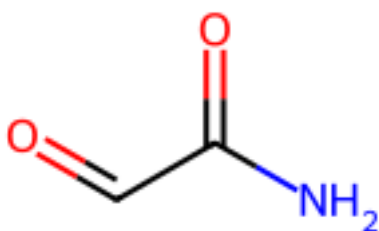## Molecule 209

SMILES: NC(=O)C=O

Molecular Formula: $C_2H_3NO_2$
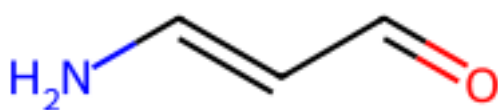
Predicted Column Density ($\log_{10}$ cm^{-2}): 13.535 ± 3.801

Molecule 210

SMILES: N/C=C/C=O

Molecular Formula: C_3H_5NO

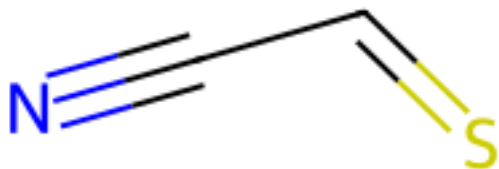Predicted Column Density ($\log_{10}$ cm^{-2}): 13.518 ± 2.218

Molecule 211

SMILES: N#CC=S

Molecular Formula: C_2HNS

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.475 ± 3.644

Molecule 212

SMILES: C=CC=CCC

Molecular Formula: C_6H_{10}

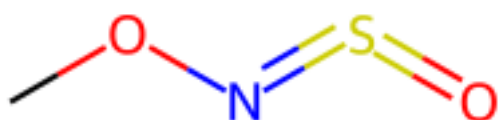Predicted Column Density ($\log_{10}$ cm^{-2}): 13.445 ± 3.807

Molecule 213

SMILES: CON=S=O

Molecular Formula: CH_3NO_2S

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.327 ± 3.883

Molecule 214

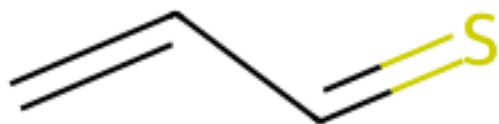SMILES: C=CC=S

Molecular Formula: C_3H_4S
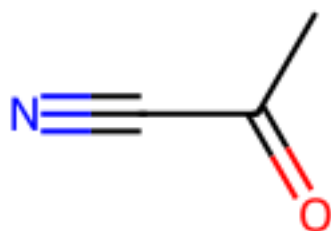
Predicted Column Density ($\log_{10}$ cm^{-2}): 13.207 ± 3.226

Molecule 215

SMILES: CC(=O)C#N

Molecular Formula: C_3H_3NO

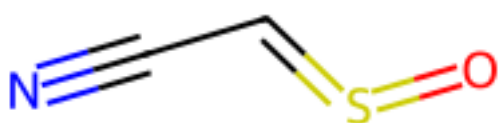Predicted Column Density ($\log_{10}$ cm^{-2}): 13.163 ± 3.413

Molecule 216

SMILES: N#CC=S=O

Molecular Formula: C_2HNOS

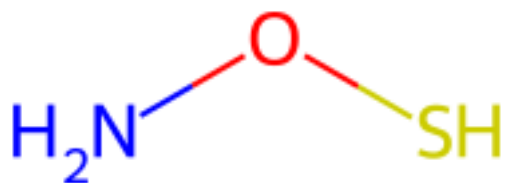Predicted Column Density ($\log_{10}$ cm^{-2}): 13.121 ± 3.609

Molecule 217

SMILES: NOS

Molecular Formula: H_3NOS

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.108 ± 3.996

Molecule 218

SMILES: O=C/C=C\C=S

Molecular Formula: C_4H_4OS

Predicted Column Density ($\log_{10}$ cm^{-2}): 13.084 ± 3.616
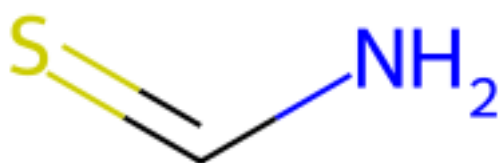

Molecule 219

SMILES: NC=S

Molecular Formula: CH_3NS

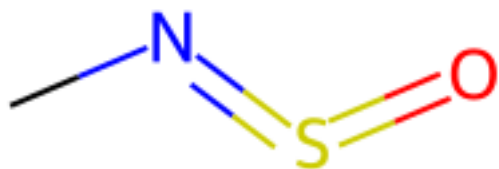Predicted Column Density ($\log_{10}$ cm^{-2}): 13.049 ± 2.724

Molecule 220

SMILES: CN=S=O

Molecular Formula: CH_3NOS

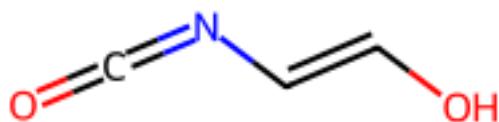Predicted Column Density ($\log_{10}$ cm^{-2}): 13.040 ± 3.652

Molecule 221

SMILES: O=C=NC=CO

Molecular Formula: $C_3H_3NO_2$

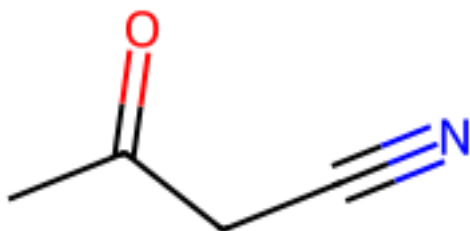Predicted Column Density ($\log_{10}$ cm^{-2}): 13.022 ± 3.941

Molecule 222

SMILES: CC(=O)CC#N

Molecular Formula: C_4H_5NO

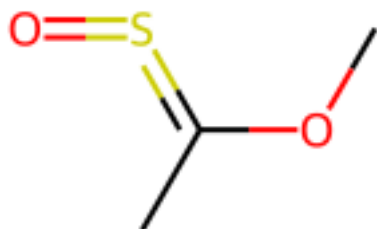Predicted Column Density ($\log_{10}$ cm^{-2}): 13.018 ± 3.924

Molecule 223

SMILES: COC(C)=S=O

Molecular Formula: $C_3H_6O_2S$

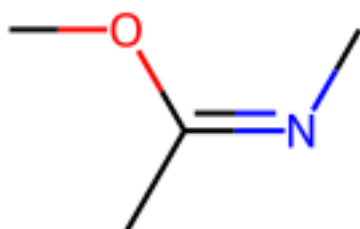Predicted Column Density ($\log_{10}$ cm^{-2}): 13.016 ± 3.682

Molecule 224

SMILES: CN=C(C)OC

Molecular Formula: C_4H_9NO

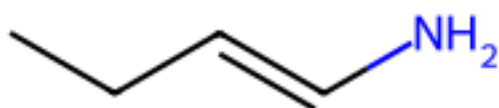Predicted Column Density ($\log_{10}$ cm^{-2}): 12.969 ± 3.935

Molecule 225

SMILES: CC/C=C/N

Molecular Formula: C_4H_9N

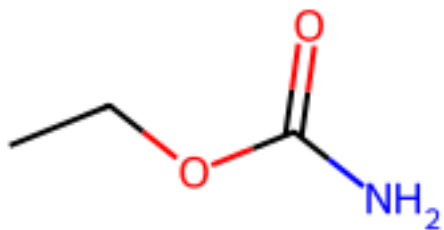Predicted Column Density ($\log_{10}$ cm^{-2}): 12.967 ± 3.519

Molecule 226

SMILES: CCOC(N)=O

Molecular Formula: $C_3H_7NO_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 12.966 ± 3.943

Molecule 227

SMILES: NC=S=O

Molecular Formula: CH_3NOS

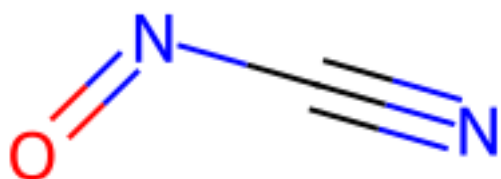Predicted Column Density ($\log_{10}$ cm^{-2}): 12.962 ± 3.149

Molecule 228

SMILES: N#CN=O

Molecular Formula: CN_2O

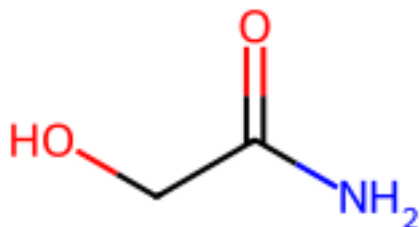Predicted Column Density ($\log_{10}$ cm^{-2}): 12.948 ± 3.222

Molecule 229

SMILES: NC(=O)CO

Molecular Formula: $C_2H_5NO_2$

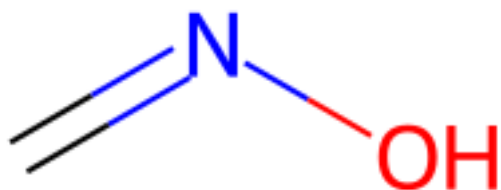Predicted Column Density ($\log_{10}$ cm^{-2}): 12.945 ± 3.876

Molecule 230

SMILES: C=NO

Molecular Formula: CH_3NO

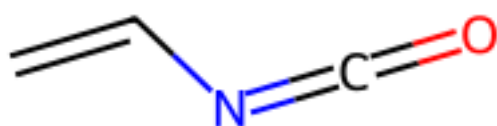Predicted Column Density ($\log_{10}$ cm^{-2}): 12.918 ± 3.890

Molecule 231

SMILES: C=CN=C=O

Molecular Formula: C_3H_3NO

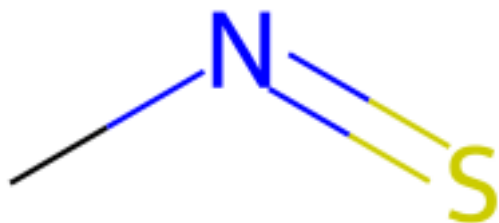Predicted Column Density ($\log_{10}$ cm^{-2}): 12.879 ± 3.821

Molecule 232

SMILES: CN=S

Molecular Formula: CH_3NS

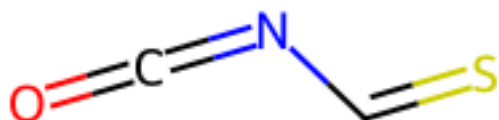Predicted Column Density (log_{10} cm^{-2}): 12.872 ± 3.788

Molecule 233

SMILES: O=C=NC=S

Molecular Formula: C_2HNOS

Predicted Column Density (log_{10} cm^{-2}): 12.849 ± 3.895

Molecule 234

SMILES: N/C=C/CC=O

Molecular Formula: C_4H_7NO

Predicted Column Density (log_{10} cm^{-2}): 12.806 ± 3.585
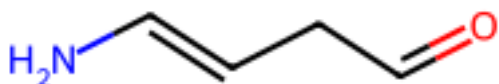
Molecule 235

SMILES: NC=CC=CO

Molecular Formula: C_4H_7NO

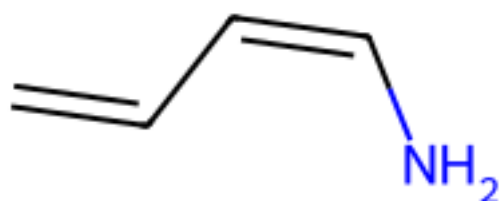Predicted Column Density ($\log_{10}$ cm^{-2}): 12.804 ± 3.789

Molecule 236

SMILES: C=C/C=C\N

Molecular Formula: C_4H_7N

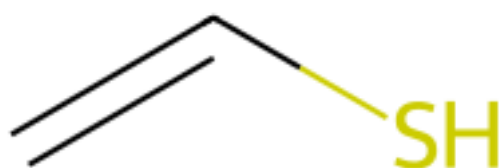Predicted Column Density ($\log_{10}$ cm^{-2}): 12.773 ± 3.280

Molecule 237

SMILES: C=CS

Molecular Formula: C_2H_4S

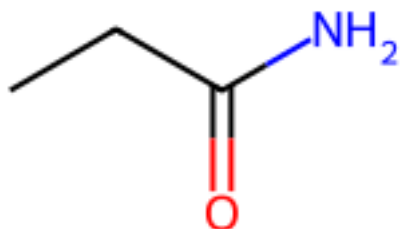Predicted Column Density ($\log_{10}$ cm^{-2}): 12.733 ± 3.104

Molecule 238

SMILES: CCC(N)=O

Molecular Formula: C_3H_7NO

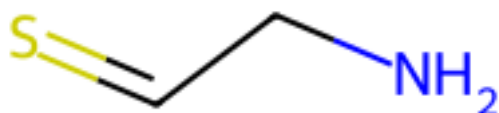Predicted Column Density ($\log_{10}$ cm^{-2}): 12.694 ± 3.439

Molecule 239

SMILES: NCC=S

Molecular Formula: C_2H_5NS

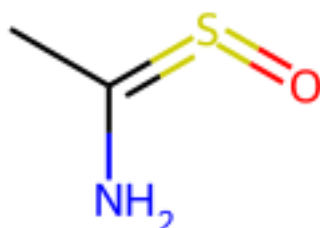Predicted Column Density ($\log_{10}$ cm^{-2}): 12.594 ± 3.967

Molecule 240

SMILES: CC(N)=S=O

Molecular Formula: C_2H_5NOS

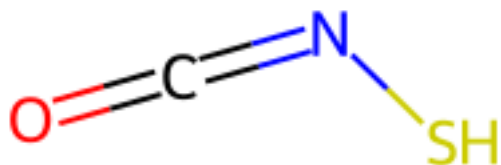Predicted Column Density ($\log_{10}$ cm^{-2}): 12.540 ± 3.941

Molecule 241

SMILES: O=C=NS

Molecular Formula: CHNOS

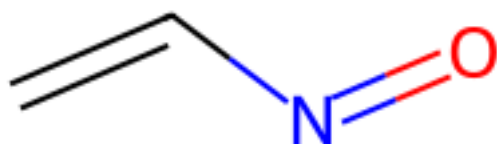Predicted Column Density ($\log_{10}$ cm^{-2}): 12.425 ± 3.271

Molecule 242

SMILES: C=CN=O

Molecular Formula: C_2H_3NO

Predicted Column Density ($\log_{10}$ cm^{-2}): 12.351 ± 3.595
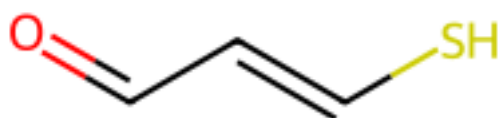
Molecule 243

SMILES: O=CC=CS

Molecular Formula: C_3H_4OS

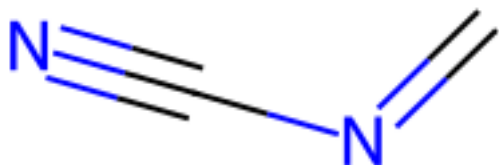Predicted Column Density ($\log_{10}$ cm^{-2}): 12.345 ± 3.486

Molecule 244

SMILES: C=NC#N

Molecular Formula: $C_2H_2N_2$

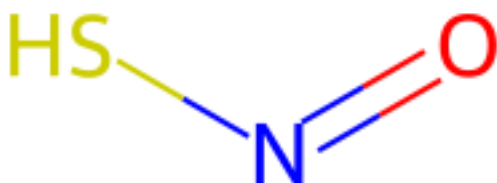Predicted Column Density ($\log_{10}$ cm^{-2}): 11.983 ± 3.841

Molecule 245

SMILES: O=NS

Molecular Formula: HNOS

Predicted Column Density ($\log_{10}$ cm^{-2}): 11.703 ± 3.432
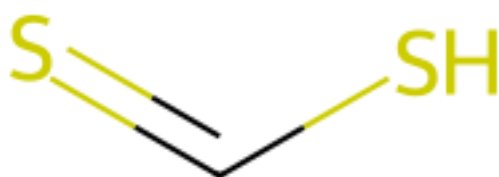
Molecule 246

SMILES: S=CS

Molecular Formula: CH_2S_2

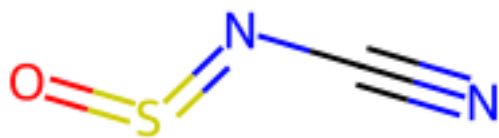Predicted Column Density ($\log_{10}$ cm^{-2}): 11.652 ± 3.992

Molecule 247

SMILES: N#CN=S=O

Molecular Formula: CN_2OS

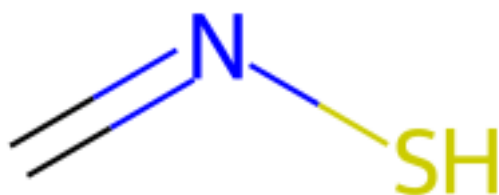Predicted Column Density ($\log_{10}$ cm^{-2}): 11.635 ± 3.936

Molecule 248

SMILES: C=NS

Molecular Formula: CH_3NS

Predicted Column Density ($\log_{10}$ cm^{-2}): 11.404 ± 3.130
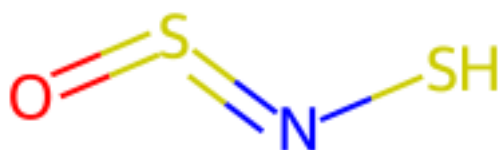

Molecule 249

SMILES: O=S=NS

Molecular Formula: $HNOS_2$

Predicted Column Density ($\log_{10}$ cm^{-2}): 10.862 ± 3.640

Molecule 250

SMILES: S=NS

Molecular Formula: HNS_2

Predicted Column Density ($\log_{10}$ cm^{-2}): 10.528 ± 3.924