NAME

>SLogPAtomTypes

SYNOPSIS

>use AtomTypes::SLogPAtomTypes;

>use AtomTypes::SLogPAtomTypes qw(:all);

DESCRIPTION

>SLogPAtomTypes class provides the following methods:

>new, AssignAtomTypes, GetAllPossibleSLogPAtomTypes, GetAllPossibleSLogPNonHydrogenAtomTypes, GetSLogPAtomTypesData, StringifySLogPAtomTypes

>The following functions are available:

>GetAllPossibleSLogPAtomTypes, GetAllPossibleSLogPNonHydrogenAtomTypes, GetSLogPAtomTypesData

>SLogPAtomTypes is derived from AtomTypes class which in turn is derived from ObjectProperty base class that provides methods not explicitly defined in SLogPAtomTypes, AtomTypes or ObjectProperty classes using Perl's AUTOLOAD functionality. These methods are generated on-the-fly for a specified object property:

```
Set<PropertyName>(<PropertyValue>);
$PropertyValue = Get<PropertyName>();
Delete<PropertyName>();
```

>The data file SLogPAomTypes.csv distributed with MayaChemTools release contains all possible SLogP [Ref 89] atom types.

>Examples of SLogP atom types:

```
C1, C2, C3, N1, N2, O1, O2 and so on
```

METHODS

>new

>>```
$NewSLogPAtomTypes = new AtomTypes::SLogPAtomTypes(%NamesAndValues);
```

>>Using specified *SLogPAtomTypes* property names and values hash, new method creates a new object and returns a reference to newly created SLogPAtomTypes object. By default, the following properties are initialized:

>>```
Molecule = ''
Type = 'SLogP'
IgnoreHydrogens = 0
```

>>Examples:

>>```
$SLogPAtomTypes = new AtomTypes::SLogPAtomTypes(
                          'Molecule' => $Molecule,
                          'IgnoreHydrogens' => 0);
```

>AssignAtomTypes

>>```
$SLogPAtomTypes->AssignAtomTypes();
```

>>Assigns SLogP atom types to all the atoms in a molecule and returns *SLogPAtomTypes*.

>GetAllPossibleSLogPAtomTypes

>>```
$AllAtomTypesDataRef = $SLogPAtomTypes->
                          GetAllPossibleSLogPAtomTypes();
$AllAtomTypesDataRef = AtomTypes::SLogPAtomTypes::
                          GetAllPossibleSLogPAtomTypes();
```

>>Returns all possible SLogP atom types corresponding to hydrogen and non-hydrogen atoms as an array

GetAllPossibleSLogPNonHydrogenAtomTypes

```
$AtomTypesDataRef = $SLogPAtomTypes->
                       GetAllPossibleSLogPNonHydrogenAtomTypes();
$AtomTypesDataRef = AtomTypes::SLogPAtomTypes::
                       GetAllPossibleSLogPNonHydrogenAtomTypes();
```

Returns all possible SLogP atom types corresponding to non-hydrogen atoms as an array reference.

GetSLogPAtomTypesData

```
$AtomTypesDataMapRef = $SLogPAtomTypes->GetSLogPAtomTypesData();
$AtomTypesDataMapRef = AtomTypes::SLogPAtomTypes::GetSLogPAtomTypesData();
```

Returns SLogP atom types and associated data loaded from SLogP data file as a reference to hash with the following hash data format:

```
@{$SLogPAtomTypesDataMap{AtomTypes}} - Array of all possible atom
                           types for all atoms
@{$SLogPAtomTypesDataMap{NonHydrogenAtomTypes}} - Array of all
                           possible atom types for non-hydrogen atoms
@{$SLogPAtomTypesDataMap->{ColLabels}} - Array of column labels
%{$SLogPAtomTypesDataMap->{DataCol<Num>}} - Hash keys pair:
                                     DataCol<Num>, AtomType
```

StringifySLogPAtomTypes

```
$String = $SLogPAtomTypes->StringifySLogPAtomTypes();
```

Returns a string containing information about *SLogPAtomTypes* object.

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SEE ALSO

AtomTypes.pm, AtomicInvariantsAtomTypes.pm, DREIDINGAtomTypes.pm, EStateAtomTypes.pm, FunctionalClassAtomTypes.pm, MMFF94AtomTypes.pm, SYBYLAtomTypes.pm, TPSAAtomTypes.pm, UFFAtomTypes.pm

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