

NAME

SLogPAtomTypes

SYNOPSIS

```
use SLogPAtomTypes;

use 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 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 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 = SLogPAtomTypes::
    GetAllPossibleSLogPAtomTypes();
```

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

`GetAllPossibleSLogPNonHydrogenAtomTypes`

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

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

`GetSLogPAtomTypesData`

```
$AtomTypesDataMapRef = $SLogPAtomTypes->GetSLogPAtomTypesData();
$AtomTypesDataMapRef = 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.

AUTHOR

Manish Sud <msud@san.rr.com>

SEE ALSO

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

COPYRIGHT

Copyright (C) 2004-2012 Manish Sud. All rights reserved.

This file is part of MayaChemTools.

MayaChemTools is free software; you can redistribute it and/or modify it under the terms of the GNU Lesser General Public License as published by the Free Software Foundation; either version 3 of the License, or (at your option) any later version.