Online data for Greenscope.

Demonstration code on GitHub at https://github.com/wbarret1/ChemicalDataSourcesTestApp

1. Obtain Chemical names/CAS Numbers.
   1. Source: NIST Webbook. They have a species list at <http://webbook.nist.gov/chemistry/download/>

This only works for exact match of chemical names.

* 1. NIH ChemSpell Web Service. Reference: <http://chemspell.nlm.nih.gov/spell/>

Call the GetSugList method on the web service. It will either return a collection of synonyms, different names with same CAS number, or a Spell Aid result, which is similar, but can contain multiple chemicals. If the Spell Aid object is returned, verify that the CAS Numbers are not the same, and the user will need to choose the chemical of interest from the list of provided chemicals.

1. ERPG Values: From AIHA publication, available online at <https://www.aiha.org/get-involved/aihaguidelinefoundation/emergencyresponseplanningguidelines/Pages/default.aspx>
2. IDLH Values: From NIOSH: <http://www.cdc.gov/niosh/idlh/intridl4.html>
3. The chemical is hazardous if it is on the List of Lists, MS Excel version available here: <http://www.epa.gov/epcra/epcracerclacaa-ss112r-consolidated-list-lists-march-2015-version>
4. TRI List: Excel spreadsheet of TRI listed chemicals: <http://www.epa.gov/toxics-release-inventory-tri-program/tri-listed-chemicals>
5. PBT List: Listed here: <http://www.epa.gov/toxics-release-inventory-tri-program/persistent-bioaccumulative-toxic-pbt-chemicals-covered-tri>
6. PUG Chem – provides molecular weight, molecular formula, and number of atoms. See <https://pubchem.ncbi.nlm.nih.gov/pug_rest/PUG_REST.html>
7. International Chemical Safety Cards (World Health Organization/NIOSH):
   1. Safety Card number from NIOSH, at <http://www.cdc.gov/niosh/ipcsneng/nengnameA.html>
   2. URL for card: "http://www.ilo.org/dyn/icsc/showcard.display?p\_lang=en&p\_card\_id=" + icscNumber + "&p\_version=1"
   3. Available Information – received in an HTML document:
      1. EC Class (Symbol)
      2. R phrase
      3. MAK
      4. Boiling Point
      5. Melting Point
      6. Density
      7. Vapor Pressure
      8. Flash Point
      9. NFPA codes
      10. Octanol/Water Partitioning Coefficient (log Kow)
   4. Values of the desired physical property were obtained using regular expressions.
8. TOXNET Hazardous Substance Database (NIH):
   1. Using TOXNET web service to search HSDB: <http://toxnet.nlm.nih.gov/toxnetapi/search_chemical.html>
   2. C# code:

First call and get temp file:

string uriString = "http://toxnet.nlm.nih.gov/cgi-bin/sis/search2";

request = (System.Net.HttpWebRequest)System.Net.WebRequest.Create(uriString);

string postData = "queryxxx=" + casNo;

postData += "&chemsyn=1";

postData += "&database=hsdb";

postData += "&Stemming=1";

postData += "&and=1";

postData += "&second\_search=1";

postData += "&gateway=1";

var data = Encoding.ASCII.GetBytes(postData);

request.Method = "POST";

request.ContentType = "application/x-www-form-urlencoded";

request.ContentLength = data.Length;

using (var stream = request.GetRequestStream())

{

stream.Write(data, 0, data.Length);

}

response = (System.Net.HttpWebResponse)request.GetResponse();

string responseString = new System.IO.StreamReader(response.GetResponseStream()).ReadToEnd();

string s1 = responseString.Replace("<br>", "");

System.Xml.XmlDocument document = new System.Xml.XmlDocument();

document.Load(new System.IO.StringReader(s1));

string tempFileName = document.FirstChild["TemporaryFile"].InnerText;

uriString = "http://toxnet.nlm.nih.gov/cgi-bin/sis/search2/f?" + tempFileName;

All chemical properties:

// Chemical Properties

request = (System.Net.HttpWebRequest)System.Net.WebRequest.Create(uriString + ":1:cpp");

response = (System.Net.HttpWebResponse)request.GetResponse();

string propertiesResposne = new System.IO.StreamReader(response.GetResponseStream()).ReadToEnd();

NOTE: On the URI for the request, replace the cpp in ":1:cpp" with:

|  |  |
| --- | --- |
| STRING | RETURNS |
| mf | Molecular Formula |
| mw | Molecular Weight |
| bp | Boiling point |
| mp | Melting point |
| den | Density |
| htc | Heat of combustion |
| htv | Heat of vaporization |
| owpc | Octanol-Water Partitioning Coefficient |
| vap | Vapor Pressure |
| ph | pH |
| auto | Auto ignition Temperature |
| csha | Chemical Safety |
| nfpa | NFPA Codes |
| etxv | Ecotoxicity Value |
| ntxv | Non-Human Toxicity Values |

Other strings are available, but these were the ones most useful for Greenscope.

* 1. Values of the desired physical property were obtained using regular expressions.

1. NIST Webbook used to obtain Heat of Formation, entropy of formation, and Cp values.
   1. Condensed phase URL:

"http://webbook.nist.gov/cgi/cbook.cgi?ID=C" + casNo.Replace("-", string.Empty) + "&Units=SI&Mask=1#Thermo-Condensed";

* 1. Gas phase URL:

"http://webbook.nist.gov/cgi/cbook.cgi?ID=C" + casNo.Replace("-", string.Empty) + "&Units=SI&Mask=1#Thermo-Gas";

* 1. Values obtained from the returned html.