



# AI4Green User Manual

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## Introduction

AI4Green is a webapp to enable synthetic organic chemists to record their work in a collaborative method, allow principal investigators and supervisors oversight of work performed, and enable synthetic pathway analysis to enable the exploration of alternative, “greener” reactions.

The AI4Green webapp functions as an electronic lab notebook (ELN) for synthetic organic chemistry and its core component is The Reaction Constructor.

We are excited to announce a beta edition of the solvent surfer has been released. Additional development to increase the number of solvents is in progress.

Future components to be added include:

1. The LCA Green Metrics Analysis
2. Route planning tool with retrosynthetic analysis, condition prediction with an integrated sustainability assessment.
3. Machine Learning driven Alternative Reaction Pathway Exploration

Note that hazard data was sourced from ECHA references on PubChem.

Details of our hazard disclaimer can be found here:

[https://ai4green.app/auth/hazard\\_disclaimer](https://ai4green.app/auth/hazard_disclaimer)

Details of our privacy notice can be found here:

[https://ai4green.app/auth/privacy\\_notice](https://ai4green.app/auth/privacy_notice)

## Getting Started

We also have a Quickstart Guide, accessible from the home page or the Help page. This is intended to help first time users with the basic functionality of AI4Green.

AI4Green can be accessed at <https://ai4green.app/> from your web browser. We highly recommend using Google Chrome.

### Registering as a New User

The first step to using the AI4Green webapp is creating an account. You will be prompted to provide a username, your full name, email address, and password.

Once registered, a user has access to the full functionality of AI4Green.

### The Home Page

After logging in, the home landing page for all users displays options for selecting, joining, and creating a workgroup. There is also a news feed displaying messages from admins.

### The Navigation Bar

The top navigation bar has links to the home page, demo reaction construction, solvent guide, a dropdown of workgroups the user is a member of, the search function, help page, and user dropdown (notifications, change hazard colours on the accessibility page, the option to login/logout, and change email/password).

The screenshot shows the AI4Green web application interface. At the top is a dark navigation bar with links: Home, Demo, Solvent Guide, Workgroup (dropdown), and Search. On the right of the bar are buttons for 'About AI4Green', 'Help', and a user profile dropdown for 'PI\_Dummy'. Below the navigation bar, a light blue banner welcomes the user 'PI\_Dummy!' and includes links for 'Learn more' and 'Quickstart Guide'. The main content area is divided into two columns. The left column, titled 'Please select a Workgroup to get started', contains a dropdown menu for selecting a workgroup and four buttons: 'Proceed to Workgroup' (green), '+ Join Existing Workgroup' (blue), '+ Create Workgroup' (blue), and 'Workgroup Membership Summary' (blue). The right column, titled 'News Feed', contains a section for 'The Solvent Surfer (Beta) is here!' with a bulleted list of features and links to get started or for help. Below this is a 'Version 1.5 Updates' section with the text 'Now available: Ketcher sketcher as a backup for marvin JS' and a link to 'Upload files to an experiment.' The footer of the page contains links for 'Hazard Disclaimer', 'Privacy Notice', 'Twitter', and 'GitHub', along with a note that hazard data is sourced from ECHA references on PubChem.

## Workgroup Structure

A workgroup is a group of users. There are three different user types with different permissions:

- Principal Investigator
- Senior Researcher
- Standard Member

After creating an account, the user will be able to join existing workgroups or create their own if they are the principal investigator/leader of a workgroup.

### Principal Investigator

When a user creates a workgroup, they will become the principal investigator of that workgroup.

Principal investigators can add/remove users from the workgroup and change their user types via the Manage Workgroup page. They can create new workbooks and add/remove users from workbooks via the Manage Workbooks page.

In a workgroup, it's possible to have multiple principal investigators. We highly recommend adding at least one additional trusted user as a principal investigator. This ensures efficient management of administrative tasks for the workgroup, particularly in situations where the primary investigator is unavailable.

### Senior Researcher

Senior Researchers can create new workbooks and add/remove users from workbooks via the Manage Workbooks page, however they cannot access the Manage Workgroup page.

### Standard Member

In the first instance of joining a workgroup, the user is set as a Standard Member. This means that they can construct and save reactions, but they cannot create new workbooks or add/remove other users.

Standard Members can submit a request to the Principal Investigator to be promoted to Senior Researcher.

Note: all users can create and save reactions.

### The Workgroup Page

The workgroup page shows the user's user type, a dropdown with the workbooks they belong to and a scrollable list of the saved reactions in that workbook.

Reactions can be sorted alphabetically or by date created. There is also the option to delete a reaction. Note that deleted reaction may not be able to be recovered.

Depending on the user type, additional options may be visible. Senior researchers and principal investigators can access Manage Workbooks and only principal investigators can access Manage Workgroups.

#### Development-Workgroup

User Type: Principal Investigator

Choose a Workbook to view or create reactions

Change Workbook

Management Workgroup

Management Workbooks

Development-Workbook

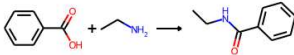
+ New Reaction

#### Your Saved Reactions

A-Z TL Date Created (Newest First) TL

Amide Coupling 1

Description of reaction.



2022-07-21 23:02:55 140833

Reload Delete

### Workbooks

Within workgroups, there are workbooks. These are collections of reactions intended to be from a single project. There can be multiple workbooks within a workgroup. All members of the workbook must belong to the workgroup too.

Once a user is a member of a workgroup and workbook they can make, save, and reload reactions and add their own novel compounds.

## Workgroup and Workbook Management

Principal investigators can manage a workgroup, and both principal investigators and senior researchers can manage workbooks.

There are two ways to change workgroup/workbook membership or user type within a workgroup:

- The principal investigator or senior researcher can do this in the “Manage Workgroup” or “Manage Workbook” pages.
- The researcher can request a change in status/access.

The screenshot shows the 'Manage Workgroup' interface. At the top, there's a navigation bar with links like Home, Demo, Help, Manage Account, Notifications, Solvent Guide, and Workgroup. Below this, the page title is 'Manage Workgroup' and the workgroup name is 'Development-Workgroup'. There are two tabs: 'Overview' and 'Requests'. The main content is a table with columns for Name, Email, and Actions. The table is divided into three sections: Principal Investigators (Pat Inglis), Senior Researchers (Sam Reed), and Standard Members (Susan Matthews). Each user row has buttons for actions like 'Promote to SR', 'Demote to SM', and 'Remove from Workgroup'.

Name	Email	Actions
<b>Principal Investigators</b>		
Pat Inglis	PI@mail.com	<button>↓ PI to SR</button> <button>Remove from Workgroup</button>
<b>Senior Researchers</b>		
Sam Reed	SR@mail.com	<button>↑ SR to PI</button> <button>↓ SR to SM</button> <button>Remove from Workgroup</button>
<b>Standard Members</b>		
Susan Matthews	SM@mail.com	<button>↑ SM to SR</button> <button>Remove from Workgroup</button>

### The Manage Workbook/Workgroup pages

The “Manage Workgroup” page allows direct promotion, demotion, and removal of users from a workgroup.

From the “Manage Workbook” page, you can remove Workbook users, or grant Workbook access to other members of the Workgroup.

Note that removal from a Workgroup also removes the user from any Workbooks of which they are members.

### Requesting changes

To request access to a Workgroup, users can select ‘Join Existing Workgroup’ from the Home Page. For access to a Workbook, the relevant button will be found on the Workgroup page.

### Accepting changes

Principal Investigators and Senior Researchers will be notified when a user makes a request. If a change has been requested, this will appear in the “Requests” tab. The approver(s) will see a link to the request page on the notification.

When a decision has been made, the requester will receive a notification on the outcome of their request

## Reaction Constructor

To build a reaction, a user must navigate to the Workgroup page. This can be done from the home page or from the “workgroup” dropdown in the navigation bar. Then a user must select the Workbook and use the “New Reaction” button.

A unique name must be specified for the reaction. Reactions are automatically saved and can be reloaded at any time from the Workgroup page.

Selected Reaction Sketcher: MarvinJS ☒ Ketcher ☐

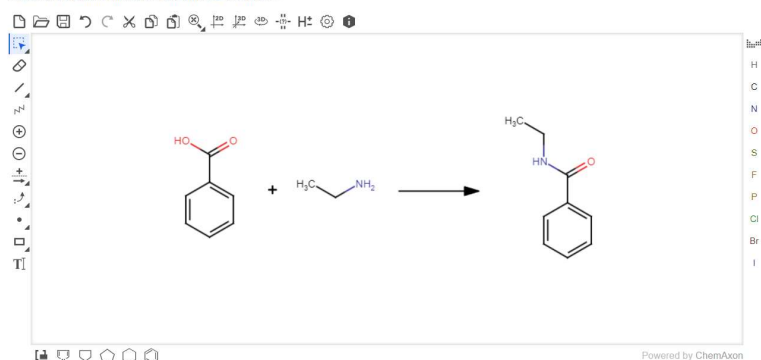


Hint: You can copy & paste reaction schemes from ChemDraw by selecting the scheme and use CTRL + ALT + C to copy and then CTRL + V to paste into this sketcher

### Using the Reaction Sketcher

There is a choice of MarvinJS or Ketcher to draw reactions. Use the tutorial button for help getting starting drawing reactions. For more detailed guidance, please refer to the MarvinJS User Manual.

Selected Reaction Sketcher: MarvinJS ☒ Ketcher ☐



Hint: You can copy & paste reaction schemes from ChemDraw by selecting the scheme and use CTRL + ALT + C to copy and then CTRL + V to paste into this sketcher

Example

Submit

## Compound Database

Once a user clicks 'Submit', the reaction drawn in the Reaction Sketcher is interpreted as SMILES strings, and the relevant molecule information (name, hazards etc.) is pulled from the PubChem database.

If a compound is not present in the PubChem database, you can add it to your workbook's Novel Compound database, where it can be accessed again. You will be prompted to provide as much information as possible regarding this compound. Once done, click 'Input'.

Reactant 1 not in database.

Name:  MW:  Hazard Codes:  CAS:  Density (g/mL):

Conc. (M):

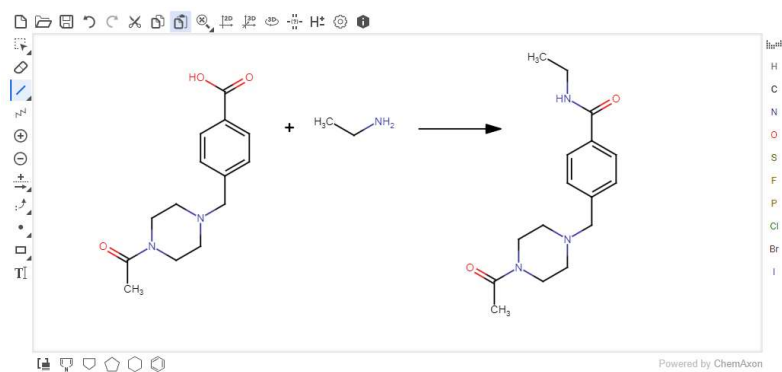
\*IUPAC names are auto-generated by [Chemical Identity Resolver](#) and [STOUT](#)

The SMILES string from the Reaction Sketcher will be used to try and generate the IUPAC name of the molecule, but this is not always possible; in which case the user must give the molecule a name.

The molecular weight will be automatically calculated and filled in. Hazard codes for novel compounds should be entered using a dash as a delimiter, e.g., 'H301-H331-H302'.

## Reaction Builder

Please sketch or upload your reaction to begin



Reactant 1 not in database.

Name:  MW:  Hazard Codes:  CAS:

Density (g/mL):  Conc. (M):



## Reaction Table

The automatically filled reaction table can now be edited. The amounts of each reactant can be adjusted, and other additions made to the reaction — solvent, reagents, and catalysts.

Any further information that is not captured by the reaction table fields can be written in the description box above the table.

### Mass, Amount, Volume

The mass of the limiting reactant can be entered, along with the equivalents of the other reactants/reagents, and from this the mass/amount/volumes are calculated. The limiting reactant always has an Equiv. of 1, and all other equivalents should be relative to this.

### Primary Reactant/Product

If there is more than one reactant, and more than one product, the circular radio buttons can be clicked to change which product and which reactant are primary. This is important for determination of yield and the final green metrics of the reaction.

### Reagents

Reagents can be searched for by entering their partial name which will return a list of reagents containing that phrase, their full name to retrieve the exact reagent or their CAS number. If no reagent is returned, it is not in the PubChem database and needs to be added via the sketcher. Depending on the entry in the PubChem database, you may need to manually enter the density of any liquids.

### Solvents

Selecting a solvent to add opens a searchable interactive dropdown. Novel Solvents can be easily added to the database in a similar way to Novel Compounds.

Here each solvent is colour coded based upon green metrics from CHEM21. Green colour means recommended solvents, yellow means problematic, red means hazardous, and maroon means highly hazardous. Solvents can also be searched for by entering their CAS number.

### Physical Form

Physical forms for each component can be entered via a dropdown menu. The selected option contributes to the risk rating of a compound, which can be viewed after pressing 'Summary'.

**Commented [JD1]:** Colour change opts

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Amide Coupling

Please describe your reaction

Please fill in the highlighted boxes to proceed

Nº	Reactants	Limiting Reagent?	Mol.Wt	Density (g/mL)	Conc. (M)	Equiv.	Amount mmol	Volume mL	Mass mg	Physical Form	Hazards
1	Benzoic Acid	<input checked="" type="radio"/>	122.12	-	-	<input type="text" value="1"/>	-	-	<input type="text" value="-select-"/>	-select-	H315-H318-H372
2	Ethylamine	<input type="radio"/>	45.08	-	-	<input type="text" value="-"/>	-	-	<input type="text" value="-select-"/>	-select-	H220-H318-H335

Catalysts/reagents

Add new reagent to database

Add Reagent

Solvents

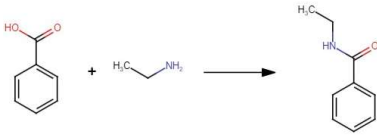
Add new solvent to database

Add Solvent

Product	Desired Product?	mmol	mg		
3 N-Ethylbenzamide	<input checked="" type="radio"/>	-	-	<input type="text" value="-select-"/>	H302

Once all relevant fields have been filled in (and these fields will be highlighted red until they have been filled), the reaction table is complete, and a summary table can be produced by clicking “Summary”.

Summary Table



Nº	Reactants/catalysts/reagents	Mol.Wt	Density (g/mL)	Conc. (M)	Equiv.	Amount (mmol)	Volume (µL)	Mass (mg)
1	Benzoic acid	122.12			1	0.82	0.00	100
2	Ethylamine	45.08	0.7		3	2.46	157	111
3	Diisopropylethylamine	129.24	0.742		1.4	1.15	200	148
4	O-(7-Azabenzotriazol-1-yl)-N,N,N',N'-tetramethyluronium hexafluorophosphate	380.23			1.2	0.98	0.00	374
Solvents							Volume (mL)	
5	Ethyl acetate						2	
Product		Mol.Wt	Theoretical Yield (mg)		Unreacted	Product Mass (mg)	% Yield	
6	N-Ethylbenzamide	149.19	122		<input type="text" value="-"/>	<input type="text" value="-"/>		

Hazards	Hazard Rating	Exposure Potential	Risk Rating
1 H315 Causes skin irritation, H318 Causes serious eye damage, H372 Causes damage to organs through prolonged or repeated exposure	VH	L	H
2 H220 Extremely flammable gas, H319 Causes serious eye irritation, H335 May cause respiratory irritation	H	H	H
3 H225 Highly Flammable liquid and vapor, H302 Harmful if swallowed, H318 Causes serious eye damage, H331 Toxic if inhaled, H335 May cause respiratory irritation	VH	M	VH
4 H228 Flammable solid, H315 Causes skin irritation, H317 May cause an allergic skin	VH	L	H

In the summary table there is safety information to fill in, information used to determine the sustainability of the reaction (using the CHEM21 green metrics), and product mass data for calculating the yield.

Sustainability (CHEM21)

Solvents

Safety

Temp °C

Elements

Batchflow

Isolation

Catalyst

Recovery

Atom Efficiency

Mass Efficiency

Yield

Conversion

Selectivity

Standard Protocols:

☐Cyclide

☐HPLC

☐Mass Spec

☐Pyrophorics

☐Microwave

☐Diazotisation

☐Hydrogenation

☐Peptide Synthesis

☐Ozone

☐Free Radicals

☐Liquid Ammonia

☐Peroxides

☐Sealed Tube

Disposal of Waste Materials:

☐Non-Halogenated Solvent

☐Halogenated Solvent

☐Specialist Container

☐Sink with Excess Water

Spillage Procedure:

☐Standard Spill Response

☐Other Spill Response (Give details on unattended experiment board)

Other Risks, controls, containment, location and PPE

(Hazardous by Products, Exothermic reactions, The need to inform others of risks, Lab and hood number )

Hazard categorisation given GLP and other controls specified

Hazard Potential to cause harm

Risk Category (A-D)

Risk Score HuRxC

Risk Likelihood of exposure

Consequences Who will be affected

Signed:

Completing a Reaction

Some fields in the Summary Table can only be completed after the reaction has been finished. Therefore, a reaction can be reloaded and fully filled out when the reaction has been completed. Note that the unreacted and product mass must be entered to mark a reaction as complete.

When a reaction is complete and all fields have been filled out, it should be locked to prevent further changes. Note that a reaction cannot be unlocked, but notes can still be added.

Add Note

×

Add a note to amend any missing or incorrect details in the reaction.

Close

Submit

Printing the Summary Table

The print summary button will allow you to print the summary table. This contains the reaction scheme & table, hazard matrix, sustainability metrics, additional hazard data, and space for the chemist’s and their supervisor’s signature.

This printout can be taken into the lab and placed near the reaction to act as a reference for the COSHH + H&S data for the reaction.

test

Reaction ID: test

Reaction Scheme

Reaction Table

Hazard Matrix

Sustainability Metrics

Standard Protocols

Other Data

Print

2 pages

Destination: Save as PDF

Pages: All

Pages per sheet: 1

Margins: Default

Options: ☒ Headers and footers, ☒ Background graphics

Colours for solvents and other metrics can be changed from the accessibility page on the user dropdown.

## Export Data

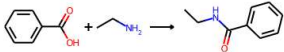
Data for a Workbook can be exported from the Workgroup page, below the list of saved reactions on the right side. There is the option to export as either a CSV file or For Print/PDF.

Your Saved Reactions


A-Z ↑ Date Created (Newest First) ↑

Amide Coupling

DW1-003



2023-03-09 14:28:05.802127

Reload  Read-only reaction created by SM\_Dummy

---

Amide-3

DW1-004

Export Reaction Data

Export as CSV Export to Print/PDF

The CSV file contains all the information from the reaction table and summary table, and all sustainability elements.

The PDF contains the name, description, time of creation and update, and summary table only.

Note that reactions updated before version 1.5 may not have all information exported.

## Solvent Guide

The solvent guide can be accessed from the top navigation bar or while building a reaction. The latter option will preload the solvent selected into the solvent guide.

№	Reactants	Limiting Reagent?	Mol.Wt	Density (g/mL)	Conc. (M)	Equiv.	Amount (mmol)	Volume (mL)	Mass (mg)	Physical Form
1	Benzoic Acid	<input checked="" type="radio"/>	122.12	-	-	<input type="text" value="1"/>	-	-	<input type="text" value=""/>	-select-
2	Ethylamine	<input type="radio"/>	45.08	-	-	<input type="text" value=""/>	-	-	<input type="text" value=""/>	-select-
Catalysts/reagents										
<input type="text" value="Add new reagent to database"/>										
Solvents										
<input type="text" value="Add new solvent to database"/>										
3	Acetic acid	<input checked="" type="radio"/>			-			<input type="text" value=""/>		-select-
Product										
<input type="text" value="Add new product to database"/>										
4	N-Ethylbenzamide	<input checked="" type="radio"/>	149.19				<input type="text" value=""/>		<input type="text" value=""/>	-select-

In the solvent guide the user can select solvents from the list on the left side of the screen which are grouped by solvent class.

These include some information about the compound including physical properties related to safety, safety, health, and environment rankings from CHEM21, and recommended substitutions.

### Solvent Guide

[About the Solvent Guide](#) [Solvent Surfer](#)

Choose up to two solvents from the classes below to compare them!

#### Acids

#### Alcohols

#### Amines

#### Aprotic polar

1,3-Dimethyl-3,4,5,6-tetrahydro-2(1H)-pyrimidinone

Acetonitrile

Dimethyl sulfoxide

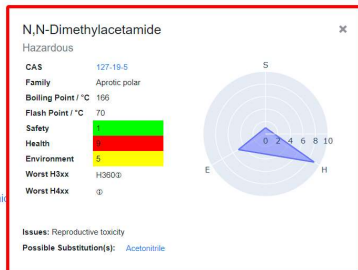
Hexamethylphosphoramide

N,N-

Dimethylacetamide

N,N-

Dimethylformamide



Information about the solvent guide can be found by pressing the “About the Solvent Guide” button.

## Search

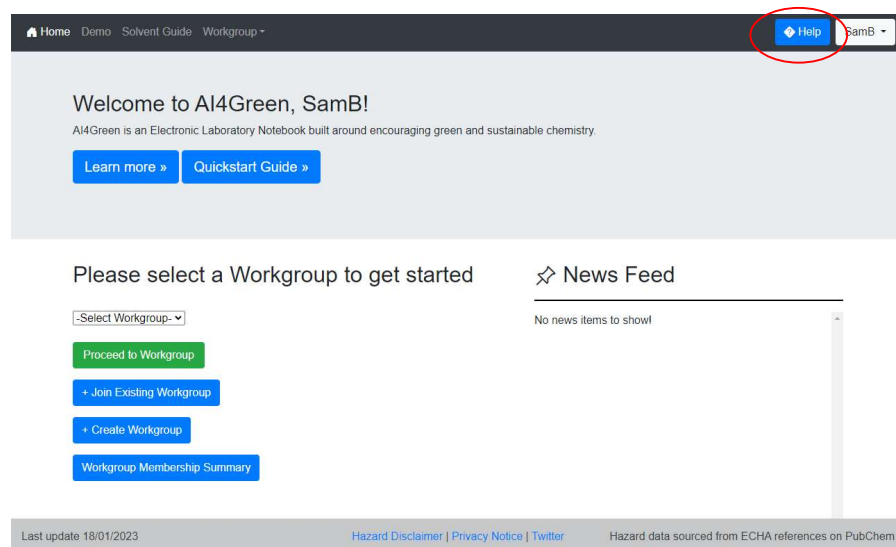
The navigation bar provides a link to the 'Search' functionality.

The user can search for structures and find all reactions from the workbooks they belong to which contain this structure. It is possible to filter the search by workgroup or workbook.

The screenshot displays the AI4Green Search interface. On the left, under 'Filters', there are dropdown menus for 'Workgroup' and 'Workbook', both currently set to 'All'. The main search area is titled 'Search reactants and products by exact structure' and shows 'Selected Reaction Sketcher: MarvinJS Ketcher'. The central canvas displays the chemical structure of benzoic acid (c1ccccc1C(=O)O). To the right of the canvas is a vertical toolbar with icons for various chemical functions. Below the canvas, a green button labeled 'Structure Search' is visible. On the right side, the 'Results' section shows '16 results found' with a table header 'A-Z | 1' and 'Date Created (Newest First) | 1'. Below the header, the number '2' is displayed, followed by the identifier 'jnw-003'. The reaction scheme shows the amide coupling of benzoic acid with ethylamine to form N-ethylbenzamide. Below the reaction, the creation and edit dates are listed: 'Created: 2023-09-18 10:57:50' and 'Edited: 2023-10-11 17:35'. There are 'Reload' and 'Delete' buttons. The reaction is labeled 'Amide coupling'.

## Further Help

Visit our help page for useful guides and video tutorials. You can also send any queries to [admin@ai4green.app](mailto:admin@ai4green.app) and a member of the team will respond to your request.



The screenshot displays the AI4Green web application interface. At the top, a dark navigation bar contains links for Home, Demo, Solvent Guide, and Workgroup. On the right side of this bar, a blue button with a white question mark icon and the text 'Help' is circled in red. Next to it is a user profile dropdown menu showing the name 'SamB'. Below the navigation bar, a light gray banner welcomes the user: 'Welcome to AI4Green, SamB!'. It includes a sub-header 'AI4Green is an Electronic Laboratory Notebook built around encouraging green and sustainable chemistry.' and two blue buttons: 'Learn more »' and 'Quickstart Guide »'. The main content area is divided into two columns. The left column, titled 'Please select a Workgroup to get started', features a dropdown menu labeled 'Select Workgroup-' and four buttons: 'Proceed to Workgroup' (green), '+ Join Existing Workgroup' (blue), '+ Create Workgroup' (blue), and 'Workgroup Membership Summary' (blue). The right column, titled 'News Feed' with a star icon, shows a message 'No news items to show!'. At the bottom, a gray footer bar contains the text 'Last update 18/01/2023', links for 'Hazard Disclaimer', 'Privacy Notice', and 'Twitter', and a note 'Hazard data sourced from ECHA references on PubChem'.