

Material property prediction

Sandia National Laboratories

Enter a SMILE string
(Multiple SMILES in new line)

Enter SMILES strings here line by line

Click to start prediction → Predict properties

Result

	smiles	Melting point	Boiling point
1	C1=CC=C(C=C1)OCC#CC#CCOC2=CC=CC=C2	367.061	565.521
2	C1=CC=C(C=C1)C#CC#CC2=CC=CC=C2	369.692	586.809
3	C1CCC(C1)(C#CC#CC2(CCCCC2)O)O	425.24	585.901
4	C1=CC=C(C=C1)C#CC2=CC=C(C=C2)	444.893	642.901
5	C#CC1=CC=CC=C1	250.34	427.457
6	CC1=C(C(CCC1)...	441.96	917.451
7	CC(=CCCC(=CC=CC(=CC=CC(=CC=...	379.794	850.478
8	CCCCCC(CC)CC1=CC(=C(C=C1#C...	443.907	913.874

Click to save the results → Save data

Predict properties

Save File

Look in: /Users/mkamruz/Desktop/Test

Name: test

Size: Kind: Date Modified

File save window

AutoSave

Home Insert Draw Page Layout Formulas Data Review View Automate

Paste

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General

Conditional Formatting

Format as Table

Cell Styles

Insert

Delete

Format

Sort & Filter

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test – Saved to my Mac

	A	B	C	D
1	smiles	MP_pred_K	BP_pred_K	
2	C1=CC=C(C=C1)OCC#CC#CCOC2=CC=CC=C2	367.06097	565.52124	
3	C1=CC=C(C=C1)C#CC#CC2=CC=CC=C2	369.6925	586.80896	
4	C1CCC(C1)(C#CC#CC2(CCCCC2)O)O	425.23965	585.9013	
5	C1=CC=C(C=C1)C#CC2=CC=C(C=C2)C#CC3=CC=CC=C3	444.8932	642.90094	
6	C#CC1=CC=CC=C1	250.33984	427.45688	
7	CC1=C(C(CCC1)(C)C=CC(=CC=CC=C(C)C=CC=C(C)C=CC2=C(CCCCC2(C)C)C)C	441.9597	917.45135	
8	CC(=CCCC(=CC=CC(=CC=CC=C(C)C=CC=C(C)C=CC=C(C)CCC=C(C)C)C)C	379.79413	850.47766	
9	CCCCCC(CC)CC1=CC(=C(C=C1#CC2=CC(=CC(=C2)C#CC3=CC(=C(C=C3CC(CC)CCCCC)C#C)CC(CC)CCC	443.9068	913.8738	
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