

# Wikidata script for SMILES, SMARTS, and CXSMILES depiction

Egon Willighagen 

Published November 12, 2022

## Citation

Willighagen, E. (2022, November 12). Wikidata script for SMILES, SMARTS, and CXSMILES depiction. *Chem-bla-ics*. <https://doi.org/10.59350/e0h5f-7cg90>

## Keywords

Wikidata, Cdk, Cxsmiles, Dagstuhl, Smiles

## Abstract

In August I reported about 2D depiction of (CX)SMILES in Wikidata via linkouts (going back to 2017). Based on a script by Magnus Manske, I wrote a Wikidata gadget that uses the same CDK Depict (VHP4Safety mirror) to depict the 2D structure in Wikidata itself:



## Copyright

Copyright © Egon Willighagen 2022. Distributed under the terms of the [Creative Commons Attribution 4.0 International License](#), which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

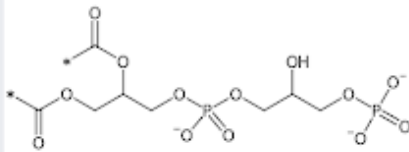
## chem-bla-ics

In August I reported about [2D depiction of \(CX\)SMILES in Wikidata via linkouts](#) (going back to 2017). Based on a script by [Magnus Manske](#), I wrote a [Wikidata gadget](#) that uses the same [CDK Depict](#) ([VHP4Safety mirror](#)) to depict the 2D structure in [Wikidata](#) itself:

**canonical SMILES**  
by Scidudebot



 OC(COP([O-])([O-])=O)COP([O-])(=O)OCC(COC([\*])=O)OC([\*])=O 

> 1 reference



+ add value

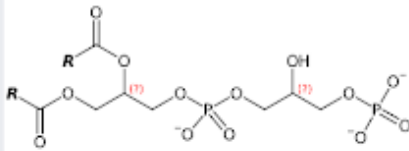
**CXSMILES**  
by Egon Willighagen

 OC(COP([O-])([O-])=O)COP([O-])(=O)OCC(COC([\*])=O)OC([\*])=O 

[S].....R.....RS

< 0 references

+ add reference



+ add value

Note the depiction of the undefined (CIP) stereochemistry on two atoms. Thanks to [Adriano](#) and [John](#) for working that out.

More about CXSMILES in Wikidata in [this Dagstuhl meeting results write up](#).