

Wikidata script for SMILES, SMARTS, and CXSMILES depiction



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Keywords

Wikidata, Cdk, Cxsmiles, Dagstuhl, Smiles



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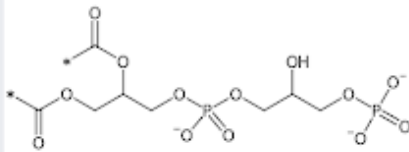
chem-bla-ics

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

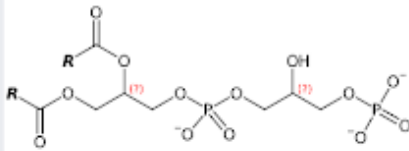
CXSMILES
by Egon Willighagen

 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](#).