

Wikidata script for SMILES, SMARTS, and CXSMILES depiction

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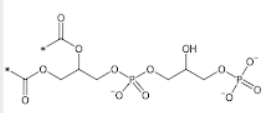
Keywords

Wikidata, Cdk, Cxsmiles, Dagstuhl, Smiles

canonical SMILES
by Scidudebot


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1 reference

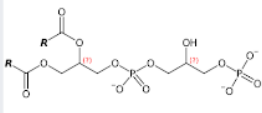


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CXSMILES
by Egon Willighagen

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0 references



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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:

Depicting of part of a Wikidata page with 2D structures of a canonical SMILES and matching CXSMILES.

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](#).