Subject: Canonical codes do not distinguish stereoisomers
Posted by wsmts on Fri, 29 Aug 2025 13:32:49 GMT
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Hi,

I noticed that for some molecules the Canonical codes don't distinguish stereoisomers even though the box was selected in the calculation dialog. (I had also deselected distinguish tautomers).

I was expecting the canonical codes to follow the pattern of the InchiKeys but they ignored the stereochemistry for these examples. (dwar attached)

v06.05.01 (Windows 11)

Best,

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Wim

File Attachments

1) Canonical Codes.dwar, downloaded 344 times