Subject: Re: Suggestion: add molecular weight calculation for individual compound
Posted by nbehrnd on Fri, 30 Jan 2026 19:22:54 GMT
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Hello Thomas

Based on Laurent's question about an explicit run to update values, I notice this does not affect _every_ value assigned by DW. As an example, while replacing benzene by triazene, for instance, I expected the "re-calculate every value, if necessary" equally would replace SMILES and InChI string, too -- which however is not the case. However, only the calculated molecular weight, and the user defined `molecular weight, rounded to two decimals) changed accordingly.

Best regards,
Norwid

File Attachments

1) 2026-01-30_DW_incomplete_re-calculate.gif, downloaded 192 times