Subject: Re: Basic Nitrogen
Posted by nbehrnd on Fri, 07 Aug 2020 15:14:46 GMT
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«Basic Nitrogen», as available under Chemistry -> From Chemical Structure -> Calculate Properties and then index card «Functional Groups» reads that the threshold applied is a pKa above 7. DW explicitly states that this a rough estimate.

The pKa estimation in the next tab, «Ionization» refers to the ChemAxon method. It is very likely that this refers to the documentation at

https://docs.chemaxon.com/display/docs/pKa_calculation.html

which include worked examples as well as literature references, too.