pK_a and pK_{aH} values of Sulfoximines from

Focus on Physico-Chemical Properties of Sulfoximines: Acidity, Basicity and Lipophilicity

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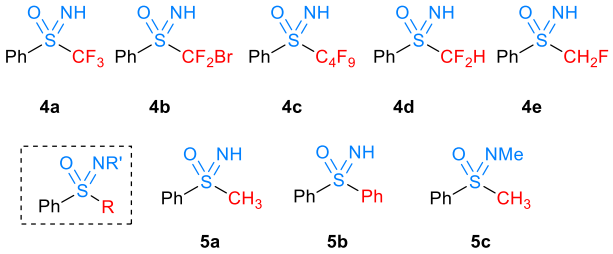
Table 2. pK_a and pK_{aH} values in MeCN of sulfoximines 4a-e, 5a-5c



	R	R'	Experimental pK_a[a]	Computed pK_a[b]	Experimental pK_{aH}[a]
4a	CF_3	H	**26.98 ± 0.12**	27.2 ± 1.2	**2.08 ± 0.10**
4b	CF_2Br	H	**27.0 ± 0.4**[c]	26.7± 1.2	**2.59 ± 0.06**
4c	C_4F_9	H	**26.48 ± 0.06**	26.3 ± 1.2	**1.24 ± 0.07**
4d	CF_2H	H		29.8 ± 1.2	**5.28 ± 0.06**
4e	CH_2F	H		31.9 ± 1.2	**7.93 ± 0.05**
5a	CH_3	H		34.9 ± 1.2	**11.24 ± 0.10**
5b	Ph	H		33.1 ± 1.2	**9.88 ± 0.05**
5c	CH_3	Me		≳40[d]	**12.32 ± 0.05**

[a] The uncertainties were evaluated to safely cover the results from measurements against different reference compounds (see the SI) and we estimate their coverage probability as approximately 80% in the context of the current pK_a and pK_{aH} scales; [b] Computationally predicted pK_a values of sulfoximines in MeCN; Details in the SI (section II.3). [c] When measuring compound **4b** some side-process(es) took place and most measurements were unsuccessful. This measurement was the only successful measurement. The nature of the compound and the sole measurement are the reason for the high uncertainty. [d] See the SI for details.