# Collection of quality-evaluated p$K_a$ values in polar aprotic solvents

**Ivo Leito, Ivari Kaljurand, Mare Piirsalu, Sofja Tshepelevitsh, Jonathan Wenyuan Zheng, Martí Rosés, Jean-François Gal**

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**Materials:** https://analytical.chem.ut.ee/cre-2026/

# Acidity of molecules in solution

The lower the p$K_a$ value the stronger the acid

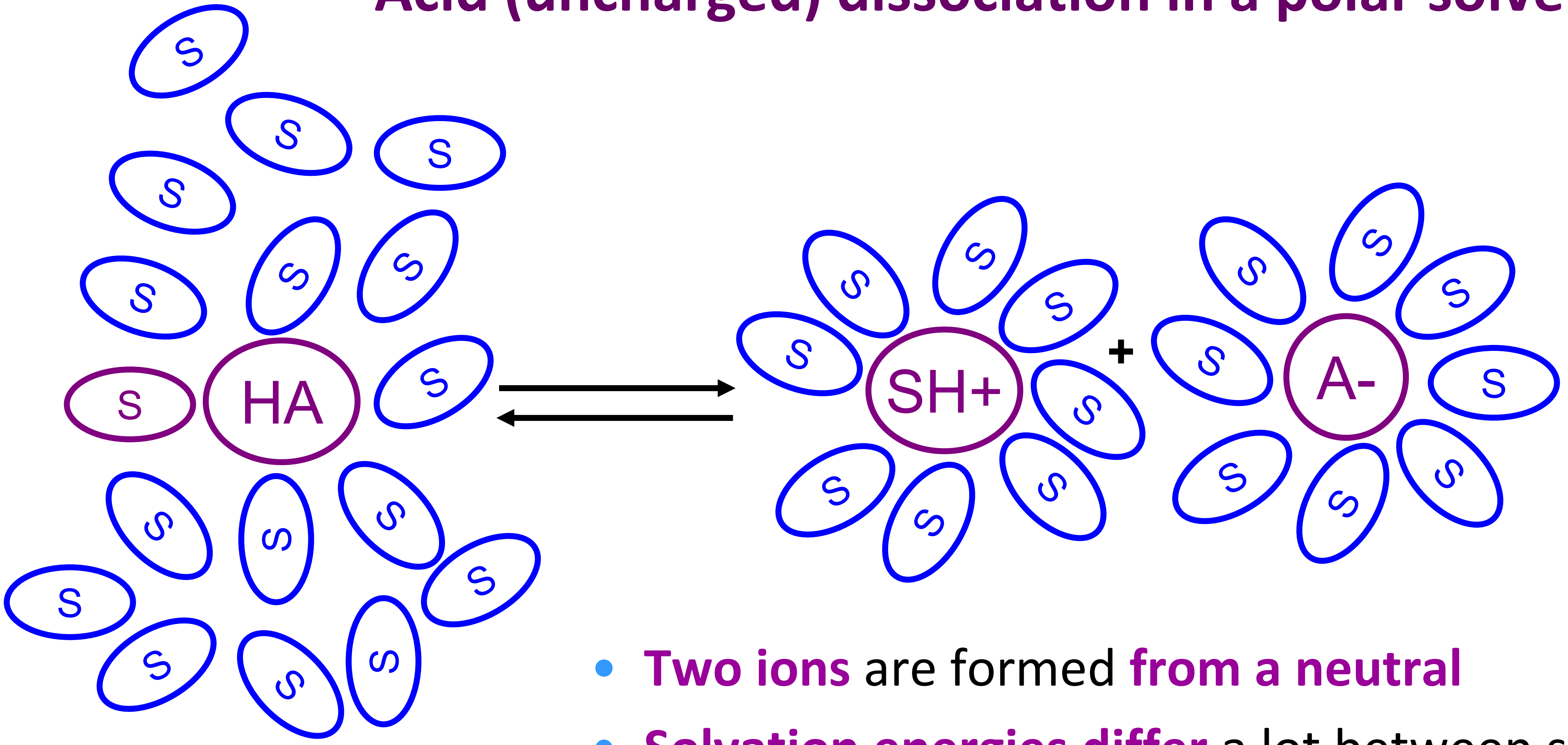
- Acidity of molecules in solution is defined in the framework of the **Brønsted** theory via the **p$K_a$ values**

$$HA + S \underset{}{\overset{K_a}{\rightleftharpoons}} A^- + SH^+$$

$$\mathrm{p}K_\mathrm{a}(\mathrm{HA}) = -\log K_\mathrm{a}(\mathrm{HA}) = -\log \frac{a(\mathrm{A}^-) \cdot a(\mathrm{SH}^+)}{a(\mathrm{HA})}$$

- Solvent S acts as a base
- Simplified scheme, valid in polar solvents
  - Ion-pairing is not considered

# Acid (uncharged) dissociation in a polar solvent




- **Two ions** are formed **from a neutral**
- **Solvation energies differ** a lot between solvents
- **p$K_a$ values** are very **solvent-sensitive**

# Example: Acetic acid

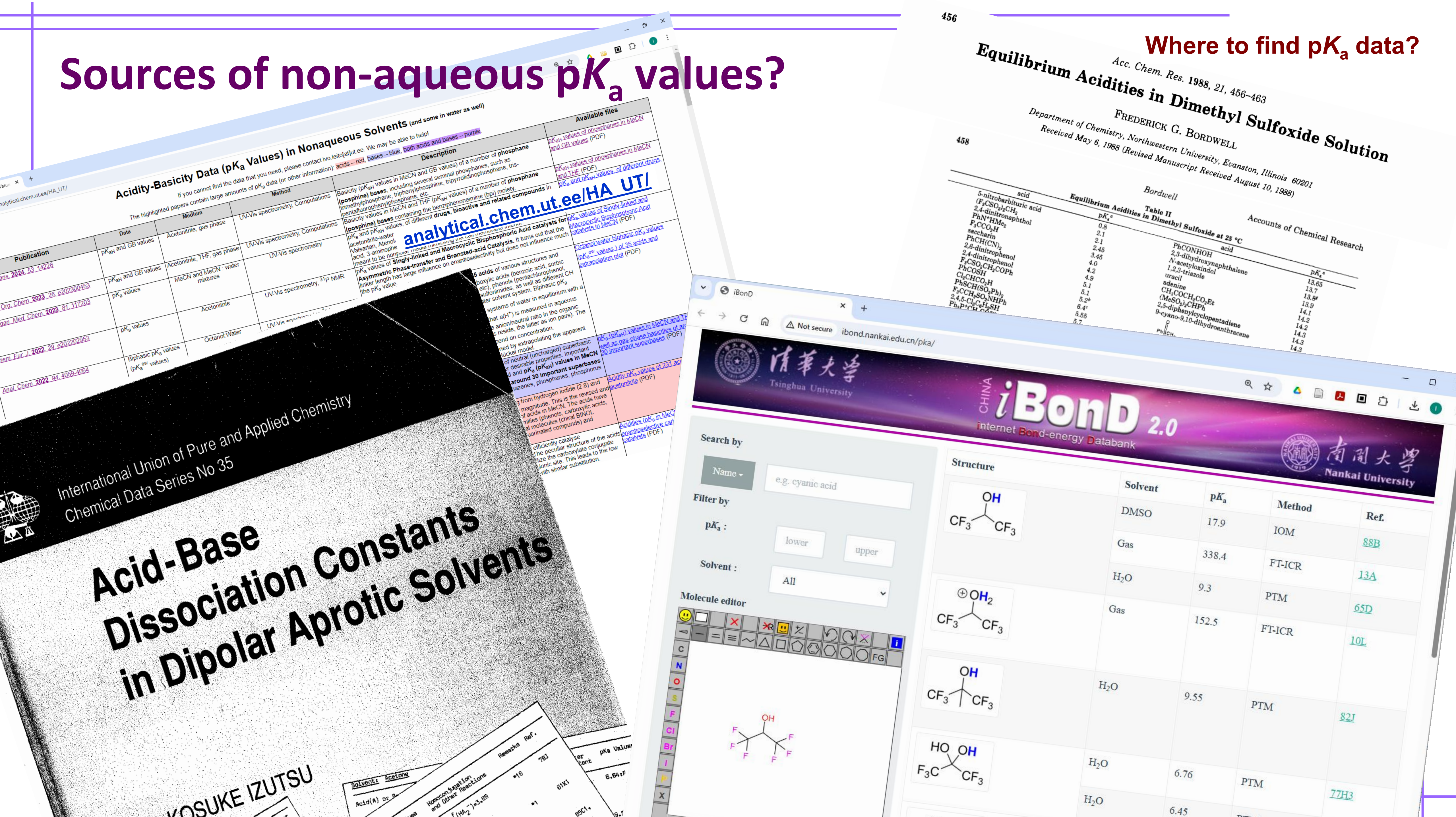
| Solvent | p$K_a$ of $CH_3COOH$ | Comments |
|---|---|---|
| THF | 24 | Approximate |
| Acetonitrile | 23.5 | |
| Propylene carbonate | 22 | Approximate |
| Acetone | 21 | Doubtful |
| Dimethylformamide | 13.5 | |
| DMSO | 12.3 | |
| Pyridine | 12 | Approximate |
| Ethanol | 10.3 | |
| Methanol | 9.6 | |
| Water | 4.76 | |

So, we need p$K_a$ data in **different** solvents

This presentation focuses on **non-aqueous solvents**

# Sources of non-aqueous p$K_a$ values?

## Where to find p$K_a$ data?



# Improvements needed?

- In available collections **data quality is not evaluated**
  - Large **discrepancies** between authors:
    - Phenol in MeCN: 26.6 .. 29.2; Fluorene in DMSO 20.5 .. 22.9; Indole in DMF: 17.6 .. 21.7; TfOH in DMSO -14.3 .. 0.5; Sulfuric acid in DMF: 3.0 .. 8.4
  - **Counterintuitive** values
    - Fluorosulfonic acid in DMF 1.6 .. 2.1; $Tf_2NH$ in DMSO 2.0 .. 2.4; Phenol in DMF 6.8
      - All these are wrong by orders of magnitude

- The available collections are
  - **not convenient for cheminformatics**
  - **not machine-readable**

# Critical compilation of acid pKa values in polar aprotic solvents

| | |
|---|---|
| **Project No.:** | 2015-020-2-500 |
| **Start Date:** | 1 May 2016 |
| **End Date:** | 25 Nov 2025 |
| **Cite:** | https://iupac.org/project/2015-020-2-500 |
| **Division:** | Analytical Chemistry Division |

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Martí Rosés
Reinhard Schwesinger
Sofja Tshepelevitsh
Jonathan Wenyuan Zheng

Objective | Description | Progress

## Objective

The objective is to summarize and critically evaluate the data on ionization constants of acids (p$K_a$ data) available in a selection of polar aprotic solvents, which are either (1) the most popular solvents for p$K_a$ determination or (2) have properties specifically suitable for determination of p$K_a$ values of certain compound classes. The outcome of the work will be a compilation together with critical evaluation of p$K_a$ values (published as an article in *Pure and Applied Chemistry*). The tentative solvent selection is the following: MeCN, DMSO, DMF, pyridine, acetone. In the polar aprotic solvents almost full coverage of measured compounds will be possible.

https://iupac.org/project/2015-020-2-500/

# Critical compilation of acid p$K_a$ values in polar aprotic solvents

- More than **9000** p$K_a$ values
- Around to **5000** acids
  - Neutral i.e. uncharged acids
  - **500+** containing F
- In **DMSO, acetonitrile, DMF, pyridine, acetone, propylene carbonate, THF**
- **Critical evaluation**
  - Around **2700** p$K_a$ values flagged as „doubtful“ or „unreliable“
  - **Corrected**, where possible: around **2400** p$K_a$ values
- Published in

*Pure and Applied Chemistry*, vol. 97, no. 9, 2025, pp. 973-998.
https://doi.org/10.1515/pac-2024-0276

- Data is freely available in Zenodo
- It is a **living database**
  - We will continue adding and correcting data

# Compound classes covered

| Acidity center | Compound class | How many* |
|---|---|---|
| **OH** | Carboxylic acids | 520 |
| | Phenols | 470 |
| | Alcohols, enols, NOH | 260 |
| | SOH, POH, AsOH, Other OH | 170 |
| **NH** | Amides, amidines, guanidines | 520 |
| | Sulfonamides, phosphonamides | 270 |
| | Aliphatic and aromatic amines | 410 |
| | Hydrazines, hydrazones, imines | 40 |
| | Heterocyclic NH acids | 600 |
| **CH** | Toluenes, di- and triphenylmethanes | 220 |
| | Other methylaromatics | 60 |
| | Cyclopentadines, indenes, fluorenes | 240 |
| | Other cyclic and heterocyclic | 140 |
| | Alkynes | 50 |
| | Esters, ketones, aldehydes, ... | 380 |
| | Sulfones, phosphanes, phosphane oxides | 270 |
| | Nitriles, Nitro | 170 |
| | Other CH | 100 |
| **Other** | SH, PH, metal hydrides, other | 180 |

** Approximate numbers of individual compounds*

# IUPAC Technical Report

DE GRUYTER

Pure Appl. Chem. 2025; 97(9): 973–998

IUPAC Technical Report

Ivo Leito*, Ivari Kaljurand, Mare Piirsalu, Sofja Tshepelevitsh, Jonathan Wenyuan Zheng, Martí Rosés and Jean-François Gal

## Acid dissociation constants in selected dipolar non-hydrogen-bond-donor solvents (IUPAC Technical Report)

https://doi.org/10.1515/pac-2024-0276
Received September 26, 2024; accepted July 2, 2025

**Abstract:** This compilation includes more than 9000 p$K_a$ values determined in seven dipolar non-hydrogen-bond-donor solvents {dimethyl sulfoxide, acetonitrile, *N,N*-dimethylformamide, pyridine, acetone, 4-methyl-1,3-dioxolan-2-one (propylene carbonate), oxolane (tetrahydrofuran)} for close to 5000 acids collected from around 800 original works published during the last 60 years. The data have been critically evaluated on the basis of defined quality criteria and depending on situation, kept as they were originally published, marked as doubtful/unreliable (around 2700 values) or corrected (around 2400 values). To enable automated processing and mining, the data are presented as a set of spreadsheets, together with structural codes (SMILES and InChI strings), compound class qualifiers, and comments. The document contains also comprehensive educational background information on the acid-base processes in non-aqueous media, as well as brief descriptions of the main measurement methods, with focus on the reliability of the data and sources of uncertainty. The full dataset is available at the permanent address https://doi.org/10.5281/zenodo.12608876.

**Keywords:** acidity; Brønsted acid; chemical equilibrium; hydrogen ion (proton) transfer; p$K_a$; solvents.

CONTENTS



- Contents:
  - Physico-chemical meaning of p$K_a$ values, definitions
  - Overview of measurement techniques, their pros and cons, sources of error
  - Overview of the data, explanations of symbols, abbreviations
  - Explanations about critical evaluation
  - Information about specific solvents
- DOI: https://doi.org/10.1515/pac-2024-0276
- Link to the p$K_a$ data in Zenodo: https://doi.org/10.5281/zenodo.12608876

Published August 15, 2025 | Version 1.4.0
Dataset Open



# Acid dissociation constants in selected dipolar non-hydrogen-bond-donor solvents

Leito, Ivo[1]; Kaljurand, Ivari[1]; Piirsalu, Mare[1]; Tshepelevitsh, Sofja[1];
Zheng, Jonathan[2]; Rosés, Martí[3]; Gal, Jean-François[4]
Show affiliations

This compilation includes more than **9000** p$K_a$ values determined in seven dipolar non-hydrogen-bond-donor solvents (dimethyl sulfoxide, acetonitrile, *N,N*-dimethylformamide, pyridine, acetone, propylene carbonate, tetrahydrofuran) for close to **5000** acids collected from around **800** original works published during the last sixty years. The data have been critically evaluated on the basis of defined quality criteria and depending on situation, kept as they were originally published, marked as doubtful/unreliable (2700 values) or corrected (around 2400 values).

To enable automated processing and mining, the data are presented as an XLSX file, together with structural codes, compound class qualifiers and comments.

**All citations should refer to the manuscript:**

> Ivo Leito, Ivari Kaljurand, Mare Piirsalu, Sofja Tshepelevitsh, Jonathan Wenyuan Zheng, Martí Rosés, Jean-François Gal. Acid Dissociation Constants in Selected Dipolar non-Hydrogen-Bond-Donor Solvents. *Pure Appl. Chem.* **2025** https://doi.org/10.1515/pac-2024-0276

## Notes

The `pKa_Dictionary.xlsx` includes thousands of embedded image files, which may cause the file to load slowly on some software/device combinations. For best results, we recommend opening the file using Microsoft Excel or LibreOffice Calc.

Versions

Version 1.4.0 Aug 15, 2025
10.5281/zenodo.16882613

Version 1.3.0 Jul 31, 2025
10.5281/zenodo.16633304

Version 1.2.0 Apr 17, 2025
10.5281/zenodo.14826175

Version 1.1.0 Dec 16, 2024
10.5281/zenodo.14502675

Version 1.0.0 Jul 28, 2024
10.5281/zenodo.12608877

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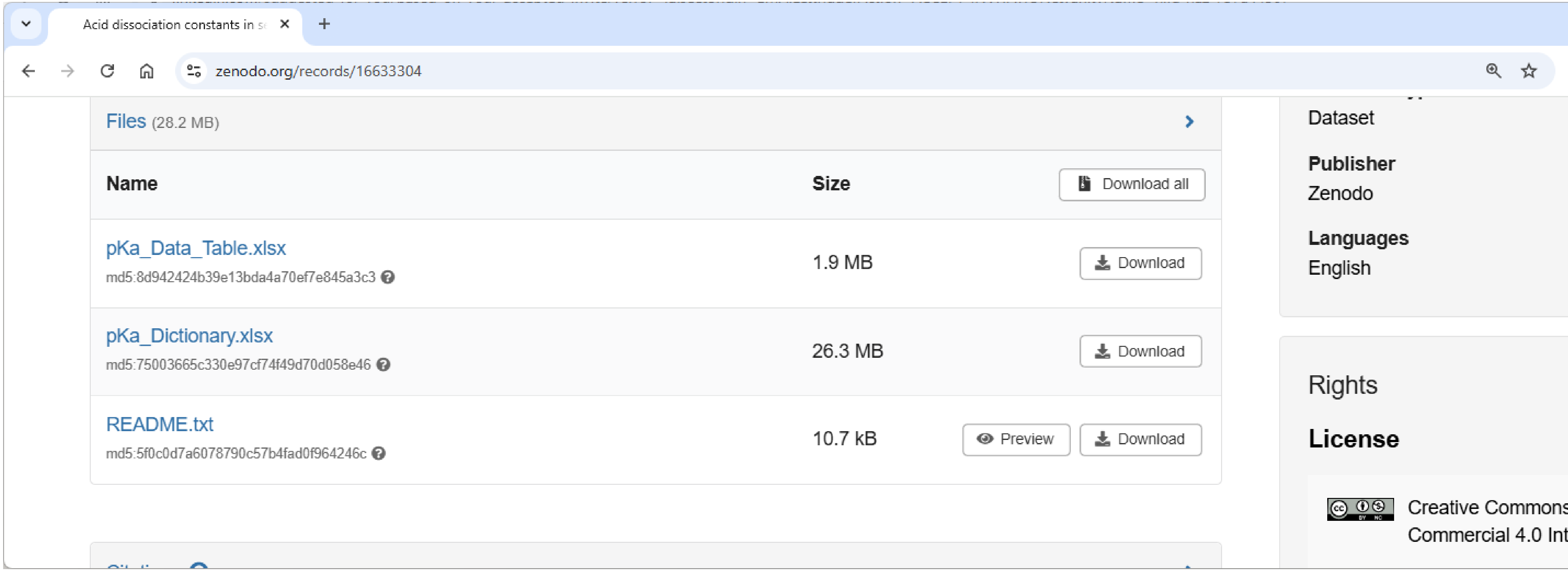
**Cite all versions?** You can cite all versions by using the DOI 10.5281/zenodo.12608876. This DOI represents all versions, and will always

# Available files



# Data table

pKa_Data_Table.xlsx [Read-Only] - Excel

F1238 | [CH3:1][c:2]1[cH:3][c:4]([N+:5](=[O:6])[O-:7])[cH:8][c:9]([N+:10](=[O:11])[O-:12])[c:13]1[OH:14]

| | Number | Compound | DMSO_p$K_a$ | DMSO_Ref | DMSO_Comments | MeCN_p$K_a$ | MeCN_Ref | MeCN_Comments | DMF_p$K_a$ | DMF_Ref | DMF_Comments | Pyridine_p$K_a$ | Pyridine_Ref | Pyridine_Comments | Acetone_p$K_a$ | Acetone_Ref | Aceton |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1231 | 1230 | 2,6-Dinitrophenol | 3.8 | K2 | C, 3 mM; doubtful | | | | 4.52 | M15 | Pot, ND; doubtful | | | | | | |
| 1232 | 1231 | 2,6-Dinitrophenol | | | | | | | 4.36 | M15 | Pot, ND; doubtful | | | | | | |
| 1233 | 1232 | 3,4-Dinitrophenol | 8.0 | C2 | Pot, 3 mM; doubtful | 18.6 | C2 | Pot; 17.92 corrected by +0.7 | | | | | | | | | |
| 1234 | 1233 | 3,4-Dinitrophenol | | | | 18.1 | M12,M13 | Pot, 17 mM; 17.65 corrected by +0.40 | | | | | | | | | |
| 1235 | 1234 | 3,5-Dinitrophenol | 10.6 | K2 | Pot, 3 mM | 22.0 | K39 | C; 20.9 corrected by +1.1 | 11.42 | C2 | Pot, 5 mM | | | | 22.7 | N4 | Pot, ND |
| 1236 | 1235 | 3,5-Dinitrophenol | | | | 21.9 | K39 | C; 20.8 corrected by +1.1 | 11.3 | K48 | Pot, ≤ 5 mM | | | | | | |
| 1237 | 1236 | 3,5-Dinitrophenol | | | | 21.5 | K2,K39,K43 | Pot; 20.5 corrected by +1.0 | | | | | | | | | |
| 1238 | 1237 | 2-Methyl-4,6-dinitrophenol | 4.6 | B21 | UV | 16.97 | K81 | UV; preferred | | | | | | | | | |
| 1239 | 1238 | 2-Methyl-4,6-dinitrophenol | | | | 17.0 | M12,M13 | Pot, 17 mM; 16.6 corrected by +0.39 | | | | | | | | | |
| 1240 | 1239 | 4-Fluoro-2,6-dinitrophenol | | | | 16.17 | K81 | UV; preferred | | | | | | | | | |
| 1241 | 1240 | 2-Chloro-4,6-dinitrophenol | | | | 14.23 | K81 | UV; preferred | | | | | | | | | |
| 1242 | 1241 | 4-Chloro-2,6-dinitrophenol | 3.7 | K1 | Pot, room temp., < 5 mM | 15.3 | K2 | Pot | | | | | | | | | |
| 1243 | 1242 | 4-Chloro-2,6-dinitrophenol | 3.6 | B2,B49 | UV; preferred | 15.0 | K43 | Pot | | | | | | | | | |
| 1244 | 1243 | 4-Chloro-2,6-dinitrophenol | 3.5 | K2 | UV, 3 mM | | | | | | | | | | | | |
| 1245 | 1244 | 4-Chloro-2,6-dinitrophenol | 3.5 | K2 | C, 3 mM | | | | | | | | | | | | |
| 1246 | 1245 | 2,4,6-Trinitrophenol (Picric acid) | -0.3 | B99 | UV, 10 mM, I → 0 | 11.0 | K45 | UV; preferred (used as anchor in K50,K8 | 3.66 | P25 | Pot, 20°C, ND, I → 0; doubtful | 3.5 | B119 | Pot, < 30 mM | 9.26 | F2 | UV, 2-5 |
| 1247 | 1246 | 2,4,6-Trinitrophenol (Picric acid) | -1.9 | K1 | UV, room temp., < 5 mM | 11.1 | K45 | UV | 3.65 | P21,P25 | Pot, ND, I → 0; doubtful | 3.0 | B119 | UV, 20°C, < 30 mM; preferre | 9.2 | F2 | Pot, 2-5 |
| 1248 | 1247 | 2,4,6-Trinitrophenol (Picric acid) | -1.0 | K2 | UV, 3 mM; approximate | 11.0 | K45,C14,K2,K39 | Pot | 3.65 | P25 | Pot, 30°C, ND, I → 0; doubtful | 2.9 | B119 | DVP, 37°C, < 30 mM | 9.2 | A11 | Pot, 7.8 |
| 1249 | 1248 | 2,4,6-Trinitrophenol (Picric acid) | 3.6 | P1 | Pot, ND, I → 0; unreliable | 10.9 | K45 | C | 3.65 | P25 | Pot, 35°C, ND; I → 0; doubtful | compl.diss. | C33 | UV, ND | 9.2 | M38 | C, 7 mM |
| 1250 | 1249 | 2,4,6-Trinitrophenol (Picric acid) | | | | 10.9 | K47 | UV, Pot | 3.64 | P25 | Pot, 40°C, ND; I → 0; doubtful | | | | 9.2 | M38 | UV, 7 m |
| 1251 | 1250 | 2,4,6-Trinitrophenol (Picric acid) | | | | 8.91 | K49 | C; doubtful | 2.9 | S16 | Pot, 28 mM; doubtful | | | | 6.3 | F9 | C, no te |
| 1252 | 1251 | 2,4,6-Trinitrophenol (Picric acid) | | | | 8.87 | K49 | UV, room temp.; doubtful | 2.2 | J4,J6 | Pot, 0.5 mM, I → 0 | | | | 9.0 | I5 | Pot, ND |
| 1253 | 1252 | 2,4,6-Trinitrophenol (Picric acid) | | | | 11.2 | P46 | UV, ND | 1.6 | K48 | UV, ≤ 5 mM; approximate | | | | 4.44 | D14 | UV, no t |
| 1254 | 1253 | 2,4,6-Trinitrophenol (Picric acid) | | | | | | | 1.2 | S15 | C, ND | | | | 3.86 | M37 | C, ND; u |
| 1255 | 1254 | 2,4,6-Trinitrophenol (Picric acid) | | | | | | | 1.1 | E5 | Pot, no temp., < 50 mM, I → 0 | | | | | | |
| 1256 | 1255 | 2,4,6-Trinitrophenol (Picric acid) | | | | | | | compl.diss. | R10 | UV, Pot, < 0.6 mM | | | | | | |

Good possibility to compare p$K_a$ values of the same acid in different solvents

pKa Data | Comments | References | Measurement uncertainty | How to cite | Statistics

# Data table

pKa_Data_Table.xlsx [Read-Only] - Excel

File | Home | Insert | Page Layout | Formulas | Data | Review | View | Help | ACROBAT | Tell me what you want to do

**For cheminformatics and machine-readability:** Canonical SMILES, Isomeric SMILES, Atom-mapped SMILES, Acidic center index, InChI, InChIKey

L1102 | B_ArOH

| | A | B | C | D | E | F | G | H | I | K | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | Number | Compound | CAS | Canonical_SMILES | omeric_SMILE | Atom-mapped_SMILES | cid_center_inde | InChI | InChIKey | Main | L1 | L2 | L3 | DMSO_p$K_a$ | DMSO_Ref | DMSO_Comments | MeCN_p$K_a$ | MeCN_Ref | MeCN_Comments |
| 1231 | 1230 | 2,6-Dinitrophenol | 573-56-8 | O=[N+]([O-])c1cccc([N+](=O)[O-])c1( | | [O:1]=[N+:2]([O-:3])[c:4]1[cH: | 13 | InChI=1/C6H4N2O5/c9- | JCRIDWXIBSEOEG-U | 1_OH | B_ArOH | A_Phenol | Nitro | 3.8 | K2 | C, 3 mM; doubtful | | | |
| 1232 | 1231 | 2,6-Dinitrophenol | 573-56-8 | O=[N+]([O-])c1cccc([N+](=O)[O-])c1( | | [O:1]=[N+:2]([O-:3])[c:4]1[cH: | 13 | InChI=1/C6H4N2O5/c9- | JCRIDWXIBSEOEG-U | 1_OH | B_ArOH | A_Phenol | Nitro | | | | | | |
| 1233 | 1232 | 3,4-Dinitrophenol | 577-71-9 | O=[N+]([O-])c1ccc(O)cc1[N+](=O)[O | | [O:1]=[N+:2]([O-:3])[c:4]1[cH: | 8 | InChI=1/C6H4N2O5/c9- | AKLOLDQYWQAREW- | 1_OH | B_ArOH | A_Phenol | Nitro | 8.0 | C2 | Pot, 3 mM; doubtful | 18.6 | C2 | Pot; 17.92 corrected by |
| 1234 | 1233 | 3,4-Dinitrophenol | 577-71-9 | O=[N+]([O-])c1ccc(O)cc1[N+](=O)[O | | [O:1]=[N+:2]([O-:3])[c:4]1[cH: | 8 | InChI=1/C6H4N2O5/c9- | AKLOLDQYWQAREW- | 1_OH | B_ArOH | A_Phenol | Nitro | | | | 18.1 | M12,M13 | Pot, 17 mM; 17.65 corr |
| 1235 | 1234 | 3,5-Dinitrophenol | 586-11-8 | O=[N+]([O-])c1cc(O)cc([N+](=O)[O-] | | [O:1]=[N+:2]([O-:3])[c:4]1[cH: | 7 | InChI=1/C6H4N2O5/c9- | UEMBNLWZFIWQFL-U | 1_OH | B_ArOH | A_Phenol | Nitro | 10.6 | K2 | Pot, 3 mM | 22.0 | K39 | C; 20.9 corrected by +1 |
| 1236 | 1235 | 3,5-Dinitrophenol | 586-11-8 | O=[N+]([O-])c1cc(O)cc([N+](=O)[O-] | | [O:1]=[N+:2]([O-:3])[c:4]1[cH: | 7 | InChI=1/C6H4N2O5/c9- | UEMBNLWZFIWQFL-U | 1_OH | B_ArOH | A_Phenol | Nitro | | | | 21.9 | K39 | C; 20.8 corrected by +1 |
| 1237 | 1236 | 3,5-Dinitrophenol | 586-11-8 | O=[N+]([O-])c1cc(O)cc([N+](=O)[O-] | | [O:1]=[N+:2]([O-:3])[c:4]1[cH: | 7 | InChI=1/C6H4N2O5/c9- | UEMBNLWZFIWQFL-U | 1_OH | B_ArOH | A_Phenol | Nitro | | | | 21.5 | K2,K39,K43 | Pot; 20.5 corrected by + |
| 1238 | 1237 | 2-Methyl-4,6-dinitrophenol | 534-52-1 | Cc1cc([N+](=O)[O-])cc([N+](=O)[O-]) | | [CH3:1][c:2]1[cH:3][c:4]([N+:5 | 14 | InChI=1/C7H6N2O5/c1- | ZXVONLUNISGICL-UH | 1_OH | B_ArOH | A_Phenol | Nitro | 4.6 | B21 | UV | 16.97 | K81 | UV; preferred |
| 1239 | 1238 | 2-Methyl-4,6-dinitrophenol | 534-52-1 | Cc1cc([N+](=O)[O-])cc([N+](=O)[O-]) | | [CH3:1][c:2]1[cH:3][c:4]([N+:5 | 14 | InChI=1/C7H6N2O5/c1- | ZXVONLUNISGICL-UH | 1_OH | B_ArOH | A_Phenol | Nitro | | | | 17.0 | M12,M13 | Pot, 17 mM; 16.6 corre |
| 1240 | 1239 | 4-Fluoro-2,6-dinitrophenol | 364-32-9 | O=[N+]([O-])c1cc(F)cc([N+](=O)[O-]) | | [O:1]=[N+:2]([O-:3])[c:4]1[cH: | 14 | InChI=1/C6H3FN2O5/c7 | MDOWEUXXLVBZIU-U | 1_OH | B_ArOH | A_Phenol | Nitro | | | | 16.17 | K81 | UV; preferred |
| 1241 | 1240 | 2-Chloro-4,6-dinitrophenol | 946-31-6 | O=[N+]([O-])c1cc(Cl)c(O)c([N+](=O)[ | | [O:1]=[N+:2]([O-:3])[c:4]1[cH: | 9 | InChI=1/C6H3ClN2O5/c | PCBCIXWBAPIVDV-UH | 1_OH | B_ArOH | A_Phenol | Nitro | | | | 14.23 | K81 | UV; preferred |
| 1242 | 1241 | 4-Chloro-2,6-dinitrophenol | 88-87-9 | O=[N+]([O-])c1cc(Cl)cc([N+](=O)[O-] | | [O:1]=[N+:2]([O-:3])[c:4]1[cH: | 14 | InChI=1/C6H3ClN2O5/c | KESYALTWUAFAAC-U | 1_OH | B_ArOH | A_Phenol | Nitro | 3.7 | K1 | Pot, room temp., < 5 mM | 15.3 | K2 | Pot |
| 1243 | 1242 | 4-Chloro-2,6-dinitrophenol | 88-87-9 | O=[N+]([O-])c1cc(Cl)cc([N+](=O)[O-] | | [O:1]=[N+:2]([O-:3])[c:4]1[cH: | 14 | InChI=1/C6H3ClN2O5/c | KESYALTWUAFAAC-U | 1_OH | B_ArOH | A_Phenol | Nitro | 3.6 | B2,B49 | UV; preferred | 15.0 | K43 | Pot |
| 1244 | 1243 | 4-Chloro-2,6-dinitrophenol | 88-87-9 | O=[N+]([O-])c1cc(Cl)cc([N+](=O)[O-] | | [O:1]=[N+:2]([O-:3])[c:4]1[cH: | 14 | InChI=1/C6H3ClN2O5/c | KESYALTWUAFAAC-U | 1_OH | B_ArOH | A_Phenol | Nitro | 3.5 | K2 | UV, 3 mM | | | |
| 1245 | 1244 | 4-Chloro-2,6-dinitrophenol | 88-87-9 | O=[N+]([O-])c1cc(Cl)cc([N+](=O)[O-] | | [O:1]=[N+:2]([O-:3])[c:4]1[cH: | 14 | InChI=1/C6H3ClN2O5/c | KESYALTWUAFAAC-U | 1_OH | B_ArOH | A_Phenol | Nitro | 3.5 | K2 | C, 3 mM | | | |
| 1246 | 1245 | 2,4,6-Trinitrophenol (Picric acid) | 88-89-1 | O=[N+]([O-])c1cc([N+](=O)[O-])c(O)c | | [O:1]=[N+:2]([O-:3])[c:4]1[cH: | 11 | InChI=1/C6H3N3O7/c1 | OXNIZHLAWKMVMX-I | 1_OH | B_ArOH | A_Phenol | Nitro | -0.3 | B99 | UV, 10 mM, I → 0 | 11.0 | K45 | UV; preferred (used as |
| 1247 | 1246 | 2,4,6-Trinitrophenol (Picric acid) | 88-89-1 | O=[N+]([O-])c1cc([N+](=O)[O-])c(O)c | | [O:1]=[N+:2]([O-:3])[c:4]1[cH: | 11 | InChI=1/C6H3N3O7/c1 | OXNIZHLAWKMVMX-I | 1_OH | B_ArOH | A_Phenol | Nitro | -1.9 | K1 | UV, room temp., < 5 mM | 11.1 | K45 | UV |
| 1248 | 1247 | 2,4,6-Trinitrophenol (Picric acid) | 88-89-1 | O=[N+]([O-])c1cc([N+](=O)[O-])c(O)c | | [O:1]=[N+:2]([O-:3])[c:4]1[cH: | 11 | InChI=1/C6H3N3O7/c1 | OXNIZHLAWKMVMX-I | 1_OH | B_ArOH | A_Phenol | Nitro | -1.0 | K2 | UV, 3 mM; approximate | 11.0 | K45,C14,K2,K39 | Pot |
| 1249 | 1248 | 2,4,6-Trinitrophenol (Picric acid) | 88-89-1 | O=[N+]([O-])c1cc([N+](=O)[O-])c(O)c | | [O:1]=[N+:2]([O-:3])[c:4]1[cH: | 11 | InChI=1/C6H3N3O7/c1 | OXNIZHLAWKMVMX-I | 1_OH | B_ArOH | A_Phenol | Nitro | 3.6 | P1 | Pot, ND, I → 0; unreliable | 10.9 | K45 | C |
| 1250 | 1249 | 2,4,6-Trinitrophenol (Picric acid) | 88-89-1 | O=[N+]([O-])c1cc([N+](=O)[O-])c(O)c | | [O:1]=[N+:2]([O-:3])[c:4]1[cH: | 11 | InChI=1/C6H3N3O7/c1 | OXNIZHLAWKMVMX-I | 1_OH | B_ArOH | A_Phenol | Nitro | | | | 10.9 | K47 | UV, Pot |
| 1251 | 1250 | 2,4,6-Trinitrophenol (Picric acid) | 88-89-1 | O=[N+]([O-])c1cc([N+](=O)[O-])c(O)c | | [O:1]=[N+:2]([O-:3])[c:4]1[cH: | 11 | InChI=1/C6H3N3O7/c1 | OXNIZHLAWKMVMX-I | 1_OH | B_ArOH | A_Phenol | Nitro | | | | 8.91 | K49 | C; doubtful |
| 1252 | 1251 | 2,4,6-Trinitrophenol (Picric acid) | 88-89-1 | O=[N+]([O-])c1cc([N+](=O)[O-])c(O)c | | [O:1]=[N+:2]([O-:3])[c:4]1[cH: | 11 | InChI=1/C6H3N3O7/c1 | OXNIZHLAWKMVMX-I | 1_OH | B_ArOH | A_Phenol | Nitro | | | | 8.87 | K49 | UV, room temp.; doubtfu |
| 1253 | 1252 | 2,4,6-Trinitrophenol (Picric acid) | 88-89-1 | O=[N+]([O-])c1cc([N+](=O)[O-])c(O)c | | [O:1]=[N+:2]([O-:3])[c:4]1[cH: | 11 | InChI=1/C6H3N3O7/c1 | OXNIZHLAWKMVMX-I | 1_OH | B_ArOH | A_Phenol | Nitro | | | | 11.2 | P46 | UV, ND |
| 1254 | 1253 | 2,4,6-Trinitrophenol (Picric acid) | 88-89-1 | O=[N+]([O-])c1cc([N+](=O)[O-])c(O)c | | [O:1]=[N+:2]([O-:3])[c:4]1[cH: | 11 | InChI=1/C6H3N3O7/c1 | OXNIZHLAWKMVMX-I | 1_OH | B_ArOH | A_Phenol | Nitro | | | | | | |
| 1255 | 1254 | 2,4,6-Trinitrophenol (Picric acid) | 88-89-1 | O=[N+]([O-])c1cc([N+](=O)[O-])c(O)c | | [O:1]=[N+:2]([O-:3])[c:4]1[cH: | 11 | InChI=1/C6H3N3O7/c1 | OXNIZHLAWKMVMX-I | 1_OH | B_ArOH | A_Phenol | Nitro | | | | | | |
| 1256 | 1255 | 2,4,6-Trinitrophenol (Picric acid) | 88-89-1 | O=[N+]([O-])c1cc([N+](=O)[O-])c(O)c | | [O:1]=[N+:2]([O-:3])[c:4]1[cH: | 11 | InChI=1/C6H3N3O7/c1 | OXNIZHLAWKMVMX-I | 1_OH | B_ArOH | A_Phenol | Nitro | | | | | | |

pKa Data | Comments | References | Measurement uncertainty | How to cite | Statistics

Ready

# Data table

**Filtered for „trifluoromethyl“**

| | Number | Compound | DMSO_pK$_a$ | DMSO_Ref | DMSO_Comments | MeCN_pK$_a$ | MeCN_Ref | MeCN_Comments | DMF_pK$_a$ | DMF_Ref | DMF_Comments | Pyridine_pK$_a$ | Pyridine_Ref | Pyridine_Comments | Acetone_pK$_a$ | Acetone_Ref | Aceton |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 845 | 844 | 2,3,4,5-Tetrabromo-6-[[[(1R,2R)-2-[[[[4-nitro-3-(t | | | | 12.7 | Z18 | UV; corrected in K81 | | | | | | | | | |
| 1094 | 1093 | 2-(Trifluoromethyl)phenol | 14.4 | K30 | Pot | 24.9 | K81 | UV; preferred | | | | | | | | | |
| 1095 | 1094 | 2-(Trifluoromethyl)phenol | | | | 24.88 | K30 | UV; corrected in K81 | | | | | | | | | |
| 1096 | 1095 | 3-(Trifluoromethyl)phenol | 15.6 | B68,B81 | UV | 26.5 | K81 | UV; preferred | 15.7 | R10 | Pot, < 0.6 mM, I ~ 1 mM | | | | | | |
| 1097 | 1096 | 3-(Trifluoromethyl)phenol | 15.1 | K30 | Pot | 26.50 | K30 | UV; corrected in K81 | | | | | | | | | |
| 1098 | 1097 | 3-(Trifluoromethyl)phenol | 14.3 | C2 | Pot, 3 mM; doubtful | 26.7 | C28 | Pot, 0.1 mM; 25.1 corrected by +1.6 | | | | | | | | | |
| 1099 | 1098 | 3-(Trifluoromethyl)phenol | | | | 26.5 | C2 | Pot; 24.9 corrected by +1.6 | | | | | | | | | |
| 1100 | 1099 | 4-(Trifluoromethyl)phenol | 15.3 | E14,R8 | UV | 25.5 | K81 | UV; preferred | | | | | | | | | |
| 1101 | 1100 | 4-(Trifluoromethyl)phenol | 15.2 | B68,B81 | UV | 25.54 | K30 | UV; corrected in K81 | | | | | | | | | |
| 1102 | 1101 | 4-(Trifluoromethyl)phenol | 14.6 | K30 | Pot | | | | | | | | | | | | |
| 1103 | 1102 | Tetrafluoro-4-(trifluoromethyl)phenol | | | | 16.6 | K81 | UV; preferred | | | | | | | | | |
| 1104 | 1103 | Tetrafluoro-4-(trifluoromethyl)phenol | | | | 16.62 | K50 | UV; corrected in K81 | | | | | | | | | |
| 1107 | 1106 | 3,5-Bis(trifluoromethyl)phenol | 13.2 | K30 | Pot | 23.8 | K81 | UV; preferred | | | | | | | | | |
| 1108 | 1107 | 3,5-Bis(trifluoromethyl)phenol | | | | 23.78 | K30 | UV; corrected in K81 | | | | | | | | | |
| 1109 | 1108 | Pentakis(trifluoromethyl)phenol | 3.1 | K30 | Pot; unreliable | 10.46 | K30,K81 | UV; preferred | | | | | | | | | |
| 1139 | 1138 | 4-Hydroxy-N-methyl-N,N-di-n-octylbenzenamini | 12.5 | S31 | UV, no temp., ND; approximate, doubtful | | | | | | | | | | | | |
| 1176 | 1175 | 4-Nitro-3-(trifluoromethyl)phenol | 9.3 | C2 | Pot, 3 mM; doubtful | 20.2 | C2 | Pot; 19.38 corrected by +0.86 | 10.38 | C2 | Pot, 5 mM | | | | | | |
| 1296 | 1295 | 4-[[4-[(Trifluoromethyl)sulfonyl]phenyl]azo]phenol | | | | | | | 12.54 | K44 | Pot, no temp., ND | | | | | | |
| 1395 | 1394 | 3-[(Trifluoromethyl)thio]phenol | 15.4 | B81,G23 | UV | | | | | | | | | | | | |
| 1396 | 1395 | 4-[(Trifluoromethyl)thio]phenol | 14.7 | B81 | UV | | | | | | | | | | | | |
| 1402 | 1401 | 3-[(Trifluoromethyl)sulfonyl]phenol | 13.2 | B81 | UV | | | | | | | | | | | | |
| 1414 | 1413 | 2,4,6-Tris[(trifluoromethyl)sulfonyl]phenol | | | | 4.44 | K81 | UV; preferred | | | | | | | | | |
| 1415 | 1414 | 2,4,6-Tris[(trifluoromethyl)sulfonyl]phenol | | | | 4.93 | K50,L13 | UV; corrected in K81 | | | | | | | | | |
| 1416 | 1415 | 2,4,6-Tris[(trifluoromethyl)sulfonyl]phenol | | | | 4.79 | L16 | UV; corrected in K81 | | | | | | | | | |
| 1417 | 1416 | 2,4,6-Tris[(trifluoromethyl)sulfonyl]phenol | | | | 4.48 | K52 | UV; corrected in K81 | | | | | | | | | |
| 1630 | 1629 | 3,3'-Bis[3,5-bis(trifluoromethyl)phenyl][1,1'-binaph | 9.7 | N13 | UV, ND | | | | | | | | | | | | |

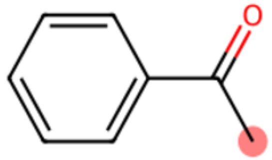
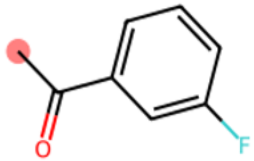
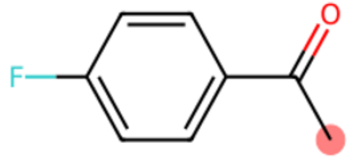
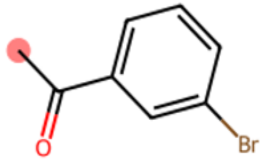
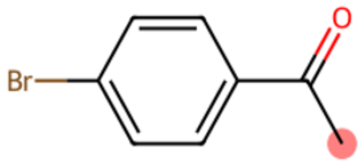
pKa Data | Comments | References | Measurement uncertainty | How to cite | Statistics

Ready 299 of 6920 records found

pKa_Dictionary.xlsx - Excel

# Dictionary file

P3238

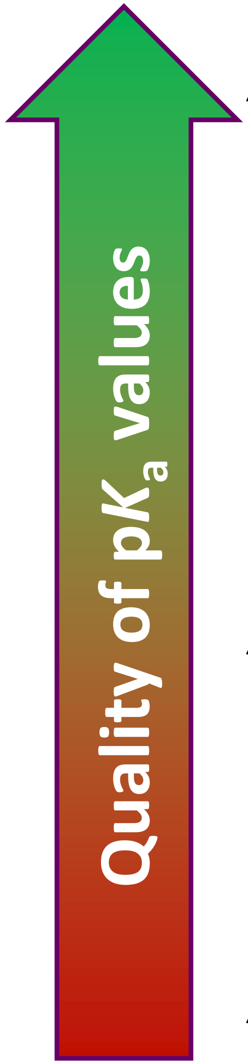
| | A | B | C | D | E | F | G | H | I | J | K | L | M | N | O | P | Q |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 3233 | 1,1,1-Trifluoro-acetone | 421-50-1 | CC(=O)C(F)(F)F | | [CH3:1][C:2](=[O:3])[C:4]([F:5])([F:6])[F:7] | 1 | InChI=1S/C3H3F3O/c1-2(7)3(4,5)6/h1H3 | InChI=1/C3H3F3O/c1-2(7)3(4,5)6/h1H3 | FHUDAMLDXFJHJE-UHFFFAOYSA-N | L23_03165 | 0 | | 1,1,1-Trifluoroacetone | [4447, 4448] |  | | |
| 3234 | Acetophenone | 98-86-2 | CC(=O)c1ccccc1 | | [CH3:1][C:2](=[O:3])[c:4]1[cH:5][cH:6][cH:7][cH:8][cH:9]1 | 1 | InChI=1S/C8H8O/c1-7(9)8-5-3-2-4-6-8/h2-6H,1H3 | InChI=1/C8H8O/c1-7(9)8-5-3-2-4-6-8/h2-6H,1H3 | KWOLFJPFCHCOCG-UHFFFAOYSA-N | L23_03166 | 0 | | Acetophenone (8Cl) | [4449, 4450, 4451] |  | | |
| 3235 | 3-Fluoro-acetophenone | 455-36-7 | CC(=O)c1cccc(F)c1 | | ](=[O:3])[c:4]1[cH:5][cH:6][cH:7][c:8]([F:9])[cH:10]1 | 1 | InChI=1S/C8H7FO/c1-6(10)7-3-2-4-8(9)5-7/h2-5H,1H3 | InChI=1/C8H7FO/c1-6(10)7-3-2-4-8(9)5-7/h2-5H,1H3 | HCEKGPAHZCYRBZ-UHFFFAOYSA-N | L23_03167 | 0 | | 3'-Fluoroacetophenone | [4452] |  | | |
| 3236 | 4-Fluoro-acetophenone | 403-42-9 | CC(=O)c1ccc(F)cc1 | | ](=[O:3])[c:4]1[cH:5][cH:6][c:7]([F:8])[cH:9][cH:10]1 | 1 | InChI=1S/C8H7FO/c1-6(10)7-2-4-8(9)5-3-7/h2-5H,1H3 | InChI=1/C8H7FO/c1-6(10)7-2-4-8(9)5-3-7/h2-5H,1H3 | ZDPAWHACYDRYIW-UHFFFAOYSA-N | L23_03168 | 0 | | 4'-Fluoroacetophenone | [4453, 4454] |  | | |
| 3237 | 3-Bromo-acetophenone | 2142-63-4 | CC(=O)c1cccc(Br)c1 | | ](=[O:3])[c:4]1[cH:5][cH:6][cH:7][c:8]([Br:9])[cH:10]1 | 1 | InChI=1S/C8H7BrO/c1-6(10)7-3-2-4-8(9)5-7/h2-5H,1H3 | InChI=1/C8H7BrO/c1-6(10)7-3-2-4-8(9)5-7/h2-5H,1H3 | JYAQYXOVOHJRCS-UHFFFAOYSA-N | L23_03169 | 0 | | 3-Bromoacetophenone | [4455] |  | | |
| 3238 | 4-Bromo-acetophenone | 99-90-1 | CC(=O)c1ccc(Br)cc1 | | ](=[O:3])[c:4]1[cH:5][cH:6][c:7]([Br:8])[cH:9][cH:10]1 | 1 | InChI=1S/C8H7BrO/c1-6(10)7-2-4-8(9)5-3-7/h2-5H,1H3 | InChI=1/C8H7BrO/c1-6(10)7-2-4-8(9)5-3-7/h2-5H,1H3 | WYECURVXVYPVAT-UHFFFAOYSA-N | L23_03170 | 0 | | p-Bromoacetophenone | [4456] |  | | |

Sheet1

Ready

# Critical evaluation

Out of **9713** values:




„Preferred“ **542**

Unflagged **6426**

„Doubtful“ **1932**

„Unreliable“ **813**

pKa_Data_Table.xlsx - Excel

E26 | 2-Hydroxy-propanoic acid (Lactic acid)

| | E | S | T | U | V | W | X | Y | Z | |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | Compound | DMSO_p$K_a$ | DMSO_Ref | DMSO_Comments | MeCN_p$K_a$ | MeCN_Ref | MeCN_Comments | DMF_p$K_a$ | DMF_Ref | DMF_Comments |
| 28 | Butanoic acid (Butyric acid) | 12.9 | C1 | Pt, 3 mM | 24.0 | C1 | Pt, 4 mM; 22.73 corrected by +1.3 | 12.5 | B109 | Pt, ND; 10.0 corrected b |
| 29 | Butanoic acid (Butyric acid) | 11.0 | B109 | Pt, ND; doubtful | | | | | | |
| 30 | 2-Methyl-propanoic acid (Isobutyric acid) | 12.8 | B101 | Pt, ND | 23.4 | B101 | Pt, ND; 22[illegible]20 corrected by +1.2, doubtful | 14.05 | B101 | Pt, ND |
| 31 | 2-Methyl-propanoic acid (Isobutyric acid) | 10.5 | B109 | Pt, ND; unreliable | | | | 13.4 | B109 | Pt, ND; 10.6 corrected b |
| 32 | 2-Methyl-propanoic acid (Isobutyric acid) | | | | | | | 4.28 | P44 | C, ND; unreliable |
| 33 | Pentanoic acid (Valeric acid) | 12.2 | B109 | Pt, ND; doubtful | | | | 13.9 | B109 | Pt, ND; 10.9 corrected b |
| 34 | 2,2-Dimethyl-propanoic acid (Pivalic acid) | 12.9 | K18 | Pt | 23.6 | B101 | Pt, ND; 22.28 corrected by +1.3, doubtful | 14.27 | B101 | Pt, ND |
| 35 | 2,2-Dimethyl-propanoic acid (Pivalic acid) | 12.9 | B101 | Pt, ND | | | | | | |
| 36 | 2,2-Dimethyl-propanoic acid (Pivalic acid) | 13.3 | F6,S1 | UV, ND; 12.4 corrected by +0.9, doubtful | | | | | | |
| 37 | Cyclohexanecarboxylic acid | | | | 24.7 | C17 | Pt; 23.3 corrected by +1.4 | | | |
| 38 | Heptanoic acid (Enanthic acid) | 11.1 | B109 | Pt, ND; doubtful | | | | 13.9 | B109 | Pt, ND; 10.9 corrected b |
| 39 | Cyclohexyl-acetic acid | 12.6 | B101 | Pt, ND | 23.3 | B101 | Pt, ND; 22.[illegible]6 corrected by +1.2, doubtful | 13.17 | B101 | Pt, ND |
| 40 | 7-Methyl-decanoic acid | | | | | | | 13.3 | E6 | Pt, ND; unreliable |
| 41 | Bicyclo[2.2.2]octane-1-carboxylic acid | 12.9 | K16,K18 | Pt | | | | | | |
| 42 | Bicyclo[2.2.2]octane-1-carboxylic acid | 12.8 | K17 | Pt, ND | | | | | | |
| 43 | Bicyclo[2.2.2]octane-1-carboxylic acid | 12.5 | R4 | Pt, 0.6 mM, I ~ 1 mM | | | | | | |
| 44 | Cubanecarboxylic acid | 12.2 | K16,K18 | Pt | | | | | | |
| 45 | Phenyl-acetic acid | 11.7 | B101 | Pt, ND | 21.8 | B101 | Pt, ND; 20[illegible]73 corrected by +1.05, doubtful | 13.5 | D1 | Pt, no temp., 10-100 mM |
| 46 | Phenyl-acetic acid | 11.6 | C4 | Pt, 10-20 mM, I = 100 mM | | | | 12.93 | B101 | Pt, ND |
| 47 | Phenyl-acetic acid | 11.6 | K18 | Pt | | | | | | |
| 48 | Phenyl-acetic acid | 10.6 | P1 | Pt, ND, I → 0; doubtful | | | | | | |
| 49 | α-Methyl-4-(2-methylpropyl)benzeneacetic acid (Ibuprofen) | | | | 22.77 | V23 | UV | | | |
| 50 | Diphenyl-acetic acid | 10.9 | R7 | UV, ~ 0.4 mM | 21.3 | B101 | Pt, ND; 20[illegible]3 corrected by +1.0, doubtful | 12.19 | B101 | Pt, ND |

In the lowest three categories: **2376** corrected values

# What was considered in critical evaluation?

- The following questions were asked:
  - Does the presented p$K_a$ value have the claimed physico-chemical meaning?
  - How was the measurement system calibrated in terms of $a(H^+)$?
  - Are the p$K_a$ values of the reference compounds close to the measured values?
  - Was the ionization ratio for the p$K_a$ calculation measured directly (from UV–VIS spectra, NMR shifts, or similar approaches)?
  - Was the concentration used sufficiently low (given the polarity of the solvent)?
  - Was the solvent appropriately purified and dried?
  - Is the p$K_a$ value within the conveniently accessible range of the chosen solvent?
  - Is difference between p$K_a$ values of the same compound in different solvents consistent with available knowledge of the solvation energies of the species present in those solvents?
  - Does the p$K_a$ value follow common chemical intuition?

# How was the measurement system calibrated in terms of $a(H^+)$?

- Typical problems:
  - Outdated p$K_a$ values used for calibrants
    - More reliable values are available
  - Measured p$K_a$ values far outside the calibration range
  - Nothing is said about calibration in the publication
  - Calibrated with aqueous buffer solutions

Corrected with reliable p$K_a$ values

Flagged „doubtful or „unreliable“

Flagged „unreliable“

# Different solvation energies → different p$K_a$ values

- The p$K_a$ differences of a compound in different solvents are first of all due to differences in three solvation energies:

Relative importance ↑

| | |
|---|---|
| $\Delta_{solv}G°(H^+,S)$ | **Highly important, main influencer** |
| $\Delta_{solv}G°(A^-,S)$ | Medium importance in **aprotic** solvents |
| $\Delta_{solv}G°(HA,S)$ | Lower importance |

- These energies are influenced by the solvent properties

# The most important is the ability to solvate $H^+$

| Solvent, S | Differencesof $\Delta_{solv}G°$ of $H^+$ from $H_2O$ (kJ/mol) |
|---|---|
| PC | +50 |
| MeCN | **+46** |
| Acetone | +29 |
| THF | 13 |
| *Water* | *0.0* |
| DMF | -14 |
| DMSO | **-19** |
| Pyridine | -28 |

Solvent basicity

Just the **different solvation of $H^+$** leads to p$K_a$ difference of around **11 p$K_a$ units**

**1 p$K_a$ unit ≡ 5.7 kJ/mol**

Y. Marcus *Ions in solution and their solvation*, Wiley, Hoboken, 2015

# Generalisations: Solvation of $H^+$

- **Solvation of $H^+$ shifts the whole p$K_a$ scale**
  - More basic solvent → lower p$K_a$
  - p$K_a$ differences of the compounds from the same family between similar solvents are often almost constant
    - Unless very special structure

You will not find an acid which has p$K_a$ in MeCN similar to Water or DMSO

p$K_a$ differences between MeCN and DMSO are typically 10 .. 13 units

Example:
p$K_a$ differences of simple **carboxylic acids**:
p$K_a$(MeCN) – p$K_a$(DMSO) ≈ 11
p$K_a$(DMF) – p$K_a$(DMSO) ≈ 1
(mostly ± 0.5)

If you find a simple carboxylic acid with p$K_a$ difference between DMSO and MeCN 5 units, one of the values is wrong with close to 100% probability

# Typical issue: no p$K_a$ data for X in solvent S

- Possible solutions:
  - **Measure**
  - **Compute**
    - Increasingly useful and used
    - Usually **correlations with experimental data** are needed for good accuracy
  - **Correlate between solvents**
    - Reliable data of **similar compounds** are needed in **both solvents**
      - Best if large span
    - Works best within a **homogeneous compound series**
    - Works best if **similar solvents**
  - **Cross-use between solvents**
    - **Only with structurally similar compounds!**
      - In many cases **acidity/basicity order** remains the same
      - Often **acidity/basicity differences** remain similar

**Kütt et al.** ***Tetrahedron Letters*** **2018,** ***59*****, 3738–3748**

EurJOC
European Journal of Organic Chemistry
Full Papers
doi.org/10.1002/ejoc.202001649

**Where to find p$K_a$ data?**

# … Sometimes published correlation equations are available

- Correlations within families work better!
  - But only for compounds belonging to the families!

Kütt et al *Eur. J. Org. Chem.* **2021**, 1407

**Table 2.** Equations for conversion of acidity data from acetonitrile to other media. Standard errors are given in parentheses. *N* – number of compounds used in regression; *S* – standard error of regression.

| Eq. No | Compounds included | *N* | Equation[a] | *S* | $R^2$ | *u*[b] | p$K_a$(MeCN) range |
|---|---|---|---|---|---|---|---|
| Water | | | | | | | |
| 1.1 | All available | 47 | $pK_a(H_2O) = pK_a(MeCN)\cdot0.72(0.03) + nC\cdot0.45(0.05) + nON\cdot0.19(0.05) - X\text{–}CO\cdot1.6(0.5) - 12.0(0.6)$ | 1.2 | 0.961 | 1.4 | 2.8…32.6 |
| 1.2 | OH acids (18 phenols, 3 carboxylic acids, 1 alcohol) | 22 | $pK_a(H_2O) = pK_a(MeCN)\cdot0.55(0.01) - X\text{–}CO\cdot2.2(0.2) + nC\cdot0.13(0.04) + MW\cdot0.0017(0.0007) - 6.5(0.5)$ | 0.3 | 0.994 | 0.3 | 4.4…29.2 |
| 1.3 | NH acids | 15 | $pK_a(H_2O) = pK_a(MeCN)\cdot0.70(0.02) - nS\cdot2.9(0.2) - nH\cdot0.24(0.06) - 3.9(0.4)$ | 0.3 | 0.995 | 0.4 | 10.5…32.6 |
| DMSO | | | | | | | |
| 2.1 | All available | 75 | $pK_a(DMSO) = pK_a(MeCN)\cdot0.94(0.02) + nHBD\cdot1.1(0.2) + X\text{-}SO2\cdot1.8(0.3) - X\text{-}H\cdot0.8(0.3) - 10.7(0.5)$ | 1.1 | 0.969 | 1.2 | 2.8…32.6 |
| 2.2 | CH acids | 27 | $pK_a(DMSO) = pK_a(MeCN)\cdot0.78(0.03) + nS\cdot1.4(0.3) - X\text{–}CN\cdot0.6(0.3) - 8.0(0.7)$ | 0.7 | 0.979 | 0.9 | 7.7…28.8 |
| 2.3 | NH acids (mainly diarylamines and sulfonamides) | 24 | $pK_a(DMSO) = pK_a(MeCN)\cdot1.00(0.02) + X\text{-}SO2\cdot2.0(0.2) + nN\cdot0.3(0.1) - 12.6(0.6)$ | 0.4 | 0.991 | 0.5 | 14.6…32.6 |
| 2.4 | OH acids (16 phenols/ naphthols, 5 other acids) | 21 | $pK_a(DMSO) = pK_a(MeCN)\cdot0.87(0.02) - nNO2\cdot1.0(0.1) + nCF3\cdot0.37(0.09) - 8.0(0.6)$ | 0.5 | 0.992 | 0.6 | 10.5…29.2 |
| DMF | | | | | | | |
| 3.1 | All available | 22 | $pK_a(DMF) = pKa(MeCN)\cdot0.91(0.03) - 7.6(0.6)$ | 0.9 | 0.982 | 0.9 | 10.2…32.6 |
| 3.2 | Phenols | 7 | $pK_a(DMF) = pKa(MeCN)\cdot0.95(0.01) - 9.5(0.3)$ | 0.2 | 0.999 | 0.2 | 11.0…29.2 |
| 3.3 | Aromatic sulfonamides | 7 | $pK_a(DMF) = pKa(MeCN)\cdot0.77(0.02) - 3.5(0.6)$ | 0.05 | 0.995 | 0.06 | 24.6…27.0 |
| DCE | | | | | | | |
| 4.1 | All available | 47 | $pK_a(DCE) = pKa(MeCN)\cdot1.10(0.03) + 32.6(0.4)$ | 1.2 | 0.973 | 1.2 | 2.8…23.5 |
| 4.2 | CH acids, excl TCNP acids[c] | 27 | $pK_a(DCE) = pK_a(MeCN)\cdot1.05(0.01) + 33.5(0.2)$ | 0.3 | 0.997 | 0.3 | 3.6…23.5 |
| 4.3 | Aromatic sulfonimides | 9 | $pK_a(DCE) = pKa(MeCN)\cdot1.03(0.03) + 32.8(0.2)$ | 0.2 | 0.995 | 0.2 | 3.3…10.0 |

# Acids, OK, but what about bases?

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## Compilation and critical evaluation of pKaH values of bases in selected dipolar non-hydrogen-bond-donor solvents

| | |
|---|---|
| **Project No.:** | 2025-017-2-500 |
| **Start Date:** | 17 Nov 2025 |
| **End Date:** | |
| **Cite:** | https://iupac.org/project/2025-017-2-500 |
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* Objective | Description | Progress

## Objective

The objective is to compile and critically evaluate the published p$K_{aH}$ values of bases in a selection of non-aqueous solvents (chosen based on the amount of published data available). The outcome of the work will be a compilation of critically evaluated (and possibly corrected) p$K_{aH}$ values, experimental metadata, and chemometric descriptors allowing the direct use of the compilation in data science and computational chemistry applications. The collected data will be analysed and described in a technical report in *Pure and Applied Chemistry* and made available in the Zenodo open-access data repository.


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# Many thanks to all of you!

**Found a mistake?**
**Your measured p$K_a$ is not in there?**
**You need a p$K_a$ that is not listed?**
**Interested in other solvent(s)?**
**Interested in p$K_{aH}$ values of bases?**

ivo.leito@ut.ee

**Slides, etc:** https://analytical.chem.ut.ee/cre-2026/