

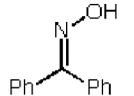
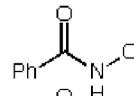
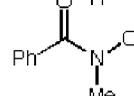
Tables des pKa

Substrate pKa H<sub>2</sub>O (DMSO)

ALCOHOLS

HOH	15.7	(27.5)
MeOH	15.54	(27.9)
<i>i</i> -PrOH	16.5	(29.3)
<i>t</i> -BuOH	17	(29.4)
<i>o</i> -hex <sub>3</sub> COH	24	
CF <sub>3</sub> CH <sub>2</sub> OH	12.5	(23.5)
(CF <sub>3</sub> ) <sub>2</sub> CHOH		(17.9)
C <sub>6</sub> H <sub>5</sub> OH	9.95	(18.0)
<i>m</i> -O <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> OH	8.35	
<i>p</i> -O <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> OH	7.14	(10.8)
<i>p</i> -OMeC <sub>6</sub> H <sub>4</sub> OH	10.20	(19.1)
2-naphthol		(17.1)

OXIMES & HYDROXAMIC ACIDS

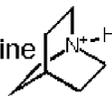
	11.3	(20.1)
	8.88	(13.7) (NH)
		(18.5)

PEROXIDES

MeOOH	11.5
CH <sub>3</sub> CO <sub>3</sub> H	8.2

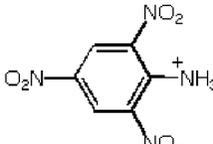
Substrate pKa H<sub>2</sub>O (DMSO)

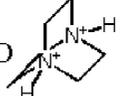
PROTONATED NITROGEN

N <sup>+</sup> H <sub>4</sub>	9.2	(10.5)
EtN <sup>+</sup> H <sub>3</sub>	10.6	
<i>i</i> -Pr <sub>2</sub> N <sup>+</sup> H <sub>2</sub>	11.05	
Et <sub>3</sub> N <sup>+</sup> H	10.75	(9.00)
PhN <sup>+</sup> H <sub>3</sub>	4.6	(3.6)
PhN <sup>+</sup> (Me) <sub>2</sub> H	5.20	(2.50)
Ph <sub>2</sub> N <sup>+</sup> H <sub>2</sub>	0.78	
2-naphthal-N <sup>+</sup> H <sub>3</sub>	4.16	
H <sub>2</sub> NN <sup>+</sup> H <sub>3</sub>	8.12	
HON <sup>+</sup> H <sub>3</sub>	5.96	
Quinuclidine 	11.0	(9.80)

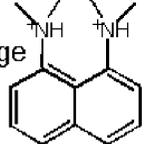
Morpholine  N<sup>+</sup>H<sub>2</sub> 8.36

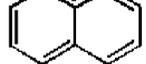
N-Me morpholine 7.38

 -9.3

DABCO  2.97, 8.82  
(2.97, 8.93)

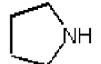
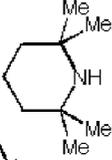
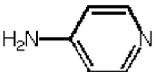
H<sub>3</sub>N<sup>+</sup>  6.90, 9.95

Proton Sponge  -9.0, 12.0  
(--, 7.50)

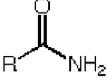
PhCN<sup>+</sup>H  -10

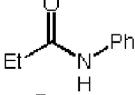
Substrate pKa H<sub>2</sub>O (DMSO)

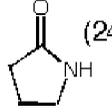
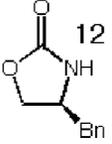
AMINES

HN <sub>3</sub>	4.7	(7.9)
NH <sub>3</sub>	38	(41)
<i>i</i> -Pr <sub>2</sub> NH		(36)
TMS <sub>2</sub> NH		(30)
PhNH <sub>2</sub>		(30.6)
Ph <sub>2</sub> NH		(25.0)
NCNH <sub>2</sub>		(16.9)
		(44)
TMP 		(37)
		(26.5)

AMIDES & CARBAMATES

		
R= H		(23.5)
CH <sub>3</sub>	15.1	(25.5)
Ph		(23.3)
CF <sub>3</sub>		(17.2)
NH <sub>2</sub> (urea)		(26.9)
OEt		(24.8)

 (21.6)

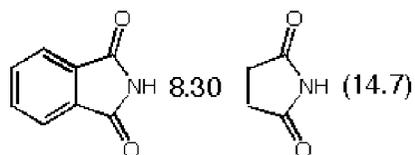
 (24.1)  12 (20.5)



Tables des pKa

Substrate pKa H<sub>2</sub>O (DMSO)

IMIDES



Ac<sub>2</sub>NH (17.9)

SULFONAMIDE

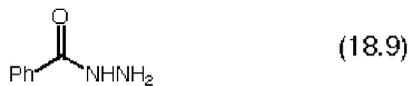
MeSO<sub>2</sub>NH<sub>2</sub> (17.5)

PhSO<sub>2</sub>NH<sub>2</sub> (16.1)

CF<sub>3</sub>SO<sub>2</sub>NH<sub>2</sub> 6.3 (9.7)

MeSO<sub>2</sub>NHPh (12.9)

GUANIDINIUM,  
HYDRAZONES, -IDES, & -INES



PhSO<sub>2</sub>NHNH<sub>2</sub> (17.2)

PhNHNHPh (26.1)

HYDROXAMIC ACID



Substrate pKa H<sub>2</sub>O (DMSO)

HYDROCARBONS

(Me)<sub>3</sub>CH 53

(Me)<sub>2</sub>CH<sub>2</sub> 51

CH<sub>2</sub>=CH<sub>2</sub> 50

CH<sub>4</sub> 48 (56)

△ 46

CH<sub>2</sub>=CHCH<sub>3</sub> 43 (44)

PhH 43

PhCH<sub>3</sub> 41 (43)

Ph<sub>2</sub>CH<sub>2</sub> 33.5 (32.2)

Ph<sub>3</sub>CH 31.5 (30.6)

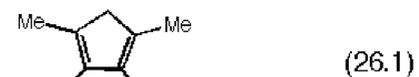
HCCH 24

PhCCH 23 (28.8)

XC<sub>6</sub>H<sub>4</sub>CH<sub>3</sub>  
X = *p*-CN (30.8)

*p*-NO<sub>2</sub> (20.4)

*p*-COPh (26.9)



H<sub>2</sub> 35

Substrate pKa H<sub>2</sub>O (DMSO)

INORGANIC ACIDS

H<sub>2</sub>O 15.7 (32)

H<sub>3</sub>O<sup>+</sup> -1.7

H<sub>2</sub>S 7.00

HBr -9.00 (0.9)

HCl -8.0 (1.8)

HF 3.17 (15)

HOCl 7.5

HClO<sub>4</sub> -10

HCN 9.4 (12.9)

HN<sub>3</sub> 4.72 (7.9)

HSCN 4.00

H<sub>2</sub>SO<sub>3</sub> 1.9, 7.21

H<sub>2</sub>SO<sub>4</sub> -3.0, 1.99

H<sub>3</sub>PO<sub>4</sub> 2.12, 7.21, 12.32

HNO<sub>3</sub> -1.3

HNO<sub>2</sub> 3.29

H<sub>2</sub>CrO<sub>4</sub> -0.98, 6.50

CH<sub>3</sub>SO<sub>3</sub>H -2.6 (1.6)

CF<sub>3</sub>SO<sub>3</sub>H -14 (0.3)

NH<sub>4</sub>Cl 9.24

B(OH)<sub>3</sub> 9.23

HOOH 11.6

Tables des pKa

Substrate	pKa	H <sub>2</sub> O (DMSO)	Substrate	pKa	H <sub>2</sub> O (DMSO)	Substrate	pKa	H <sub>2</sub> O (DMSO)	
<b>KETONES</b>						<b>AMIDINES</b>			
X= H		(26.5)	X= H		(24.7)	R= Me		(17.3)	
Ph		(19.8)	OMe		(25.7)	Ph		(15.0)	
SPh		(18.7)	NMe <sub>2</sub>		(27.5)	<b>PROTONATED HETEROCYCLES</b>			
COCH <sub>3</sub>	9	(13.3)	Br		(23.8)	<b>DBU</b> (11-12)			
SO <sub>2</sub> Ph		(15.1)	CN		(22.0)	(estimate)			
	19-20	(27.1)				<b>DMAP</b>			
		(28.3)	n= 4		(25.1)	9.2		6.95	
		(27.7)	5		(25.8)				
		(26.3)	6		(26.4)	R= H (PPTS)	5.21	(3.4)	
		(26.3)	7		(27.7)	t-Bu	4.95	(0.90)	
			8		(27.4)	Me	6.75	(4.46)	
X= H		(24.7)			(28.1)	Cl, H	0.72		
CH <sub>3</sub>		(24.4)			(29.0)	<b>HETEROCYCLES</b>			
Ph		(17.7)			(25.5)				
COCH <sub>3</sub>		(12.7)			(25.5)	(20.95)			
COPh		(13.3)			(32.4)		(23.0)		(18.6)
CO <sub>2</sub> Et		(22.7)				<b>1,2,3 triazole</b>			
CN		(10.2)					(17.0)		(13.9)
F		(21.6)							
OMe		(22.85)							
OPh		(21.1)							
SPh		(16.9)							
SePh		(18.6)							
NPh <sub>2</sub>		(20.3)							
N <sup>+</sup> Me <sub>3</sub>		(14.6)							
NO <sub>2</sub>		(7.7)							
SO <sub>2</sub> Ph		(11.4)							

Tables des pKa

Substrate pKa H<sub>2</sub>O (DMSO)

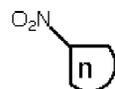
NITRILES		
X= H		(31.3)
CH <sub>3</sub>		(32.5)
Ph		(21.9)
COPh		(10.2)
CONR <sub>2</sub>		(17.1)
CO <sub>2</sub> Et		(13.1)
CN	11	(11.1)
OPh		(28.1)
N <sup>+</sup> Me <sub>3</sub>		(20.6)
SPh		(20.8)
SO <sub>2</sub> Ph		(12.0)

HETERO-AROMATICS

	(28.2)
	(30.1)
	(26.7)
	(25.2)
	(30.2)
	(30.0)

Substrate pKa H<sub>2</sub>O (DMSO)

NITRO		
RNO <sub>2</sub>		
R= CH <sub>3</sub>	≈10	(17.2)
CH <sub>2</sub> Me		(16.7)
CHMe <sub>2</sub>		(16.9)
CH <sub>2</sub> Ph		(12.2)
CH <sub>2</sub> Bn		(16.2)
CH <sub>2</sub> SPh		(11.8)
CH <sub>2</sub> SO <sub>2</sub> Ph		(7.1)
CH <sub>2</sub> COPh		(7.7)



n= 3	(26.9)
4	(17.8)
5	(16.0)
6	(17.9)
7	(15.8)

IMINES



Substrate pKa H<sub>2</sub>O (DMSO)

SULFOXIDES		
X= H		(35.1)
Ph		(29.0)
SPh		(29.0)
X= H		(33)
Ph		(27.2)
SOPh		(18.2)
		(24.5)

SULFONIUM

Me <sub>3</sub> S <sup>+</sup> =O	(18.2)
	(16.3)

SULFIMIDES & SULFOXIMINES

R= Me	(27.6)
iPr	(30.7)
	(24.5)
	(33)
	(14.4)
	(20.7)

Tables des pKa

Substrate pKa H<sub>2</sub>O (DMSO)

PHOSPHONIUM

P <sup>+</sup> H <sub>4</sub>	-14
MeP <sup>+</sup> H <sub>3</sub>	2.7
Et <sub>3</sub> P <sup>+</sup> H	9.1
Ph <sub>3</sub> P <sup>+</sup> CH <sub>3</sub>	(22.4)
Ph <sub>3</sub> P <sup>+</sup> <i>i</i> Pr	(21.2)
Ph <sub>3</sub> P <sup>+</sup> CH <sub>2</sub> COPh	(6.2)
Ph <sub>3</sub> P <sup>+</sup> CH <sub>2</sub> CN	(7.0)

PHOSPONATES & PHOSPHINE OXIDES

X= Ph	(27.6)
CN	(16.4)
CO <sub>2</sub> Et	(18.6)
Cl	(26.2)
SiMe <sub>3</sub>	(28.8)
X= SPh	(24.9)
CN	(16.9)

PHOSPHINES

Ph <sub>2</sub> PCH <sub>2</sub> PPh <sub>2</sub>	(29.9)
Ph <sub>2</sub> PCH <sub>2</sub> SO <sub>2</sub> Ph	(20.3)

Substrate pKa H<sub>2</sub>O (DMSO)

PROTONATED SPECIES

	-12.4
	-7.8
	-6.2
	-6.5
	-3.8
	-2.05
MeOH <sub>2</sub> <sup>+</sup>	-2.2
	-1.8
	0.79

SULFINIC & SULFONIC ACIDS

	-2.6
	7.1

Substrate pKa H<sub>2</sub>O (DMSO)

SULFIDES

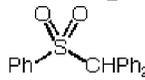
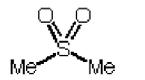
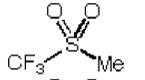
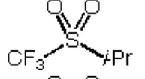
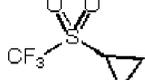
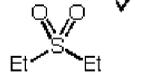
PhSCH <sub>2</sub> X	
X= Ph	(30.8)
CN	(20.8)
COCH <sub>3</sub>	(18.7)
COPh	(16.9)
NO <sub>2</sub>	(11.8)
SPh	(30.8)
SO <sub>2</sub> Ph	(20.3)
SO <sub>2</sub> CF <sub>3</sub>	(11.0)
POPh <sub>2</sub>	(24.9)
MeSCH <sub>2</sub> SO <sub>2</sub> Ph	(23.4)
PhSCHPh <sub>2</sub>	(26.7)
(PhS) <sub>3</sub> CH	(22.8)
(PrS) <sub>3</sub> CH	(31.3)
	(30.5)
(PhS) <sub>2</sub> CHPh	(23.0)
X= Ph	(30.7)
CO <sub>2</sub> Me	(20.8)
CN	(19.1)
RSCH <sub>2</sub> CN	
R= Me	(24.3)
Et	(24.0)
<i>i</i> Pr	(23.6)
<i>t</i> -Bu	(22.9)
PhSCH=CHCH <sub>2</sub> SPh	(26.3)
BuSH	10-11 (17.0)
PhSH	≈7 (10.3)

## Tables des pKa

Substrate pKa H<sub>2</sub>O (DMSO)

### SULFONES



X= H	(29.0)
CH <sub>3</sub>	(31.0)
<i>t</i> -Bu	(31.2)
Ph	(23.4)
CH=CH <sub>2</sub>	(22.5)
CH=CHPh	(20.2)
CCH	(22.1)
CCPh	(17.8)
COPh	(11.4)
COMe	(12.5)
OPh	(27.9)
N <sup>+</sup> Me <sub>3</sub>	(19.4)
CN	(12.0)
NO <sub>2</sub>	(7.1)
SMe	(23.5)
SPh	(20.5)
SO <sub>2</sub> Ph	(12.2)
PPh <sub>2</sub>	(20.2)
	(22.3)
	(31.1)
	(18.8)
	(21.8)
	(26.6)
	(32.8)
(PhSO <sub>2</sub> ) <sub>2</sub> CH <sub>2</sub> Me	(14.3)

DMSO:

JACS 97, 7007 (1975)  
 JACS 97, 7160 (1975)  
 JACS 97, 442 (1975)  
 JACS 105, 6188 (1983)  
 JOC 41, 1883 (1976)  
 JOC 41, 1885 (1976)  
 JOC 41, 2786 (1976)  
 JOC 41, 2508 (1976)  
 JOC 42, 1817 (1977)  
 JOC 42, 321 (1977)  
 JOC 42, 326 (1977)  
 JOC 43, 3113 (1978)  
 JOC 43, 3095 (1978)  
 JOC 43, 1764 (1978)  
 JOC 45, 3325 (1980)  
 JOC 45, 3305 (1980)  
 JOC 45, 3884 (1980)  
 JOC 46, 4327 (1981)  
 JOC 46, 632 (1981)  
 JOC 47, 3224 (1982)  
 JOC 47, 2504 (1982)  
 Acc. Chem. Res. 21, 456 (1988)  
 Unpublished results of F. Bordwell

Water:

Advanced Org. Chem., 3rd Ed.  
 J. March (1985)  
 Unpublished results of W. P. Jencks

THF:

JACS 110, 5705 (1988)