

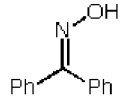
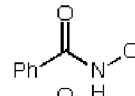
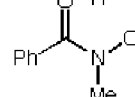
Tables des pKa

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

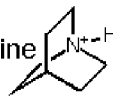
	11.3	(20.1)
	8.88	(13.7) (NH)
		(18.5)


PEROXIDES

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

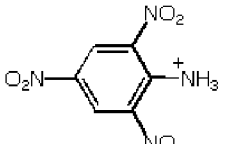
Substrate pKa H<sub>2</sub>O (DMSO)

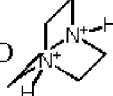
PROTONATED NITROGEN

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)

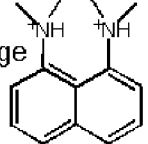
Morpholine  N<sup>+</sup>H<sub>2</sub> 8.36

N-Me morpholine 7.38

 -9.3

DABCO  2.97, 8.82  
(2.97, 8.93)


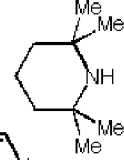
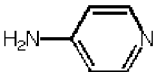
H<sub>3</sub>N<sup>+</sup>  6.90, 9.95

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

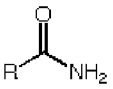
PhCN<sup>+</sup>H  -10

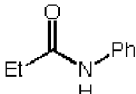
Substrate pKa H<sub>2</sub>O (DMSO)

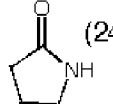
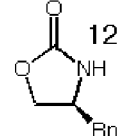
AMINES

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)
CARBOXYLIC ACIDS		
X= CH <sub>3</sub>	4.76	(12.3)
CH <sub>2</sub> NO <sub>2</sub>	1.68	
CH <sub>2</sub> F	2.66	
CH <sub>2</sub> Cl	2.86	
CH <sub>2</sub> Br	2.86	
CH <sub>2</sub> I	3.12	
CHCl <sub>2</sub>	1.29	
CCl <sub>3</sub>	0.65	
CF <sub>3</sub>	-0.25	
H	3.77	
HO	3.6, 10.3	
C <sub>6</sub> H <sub>5</sub>	4.2	(11.1)
<i>o</i> -O <sub>2</sub> NC <sub>6</sub> H <sub>4</sub>	2.17	
<i>m</i> -O <sub>2</sub> NC <sub>6</sub> H <sub>4</sub>	2.45	
<i>p</i> -O <sub>2</sub> NC <sub>6</sub> H <sub>4</sub>	3.44	
<i>o</i> -ClC <sub>6</sub> H <sub>4</sub>	2.94	
<i>m</i> -ClC <sub>6</sub> H <sub>4</sub>	3.83	
<i>p</i> -ClC <sub>6</sub> H <sub>4</sub>	3.99	
<i>o</i> -(CH <sub>3</sub> ) <sub>3</sub> N <sup>+</sup> C <sub>6</sub> H <sub>4</sub>	1.37	
<i>p</i> -(CH <sub>3</sub> ) <sub>3</sub> N <sup>+</sup> C <sub>6</sub> H <sub>4</sub>	3.43	
<i>p</i> -OMeC <sub>6</sub> H <sub>4</sub>	4.47	
R= H	4.25	
<i>trans</i> -CO <sub>2</sub> H	3.02, 4.38	
<i>cis</i> -CO <sub>2</sub> H	1.92, 6.23	

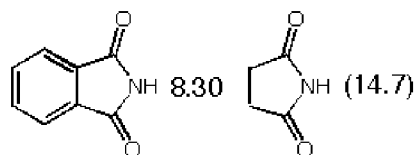
Substrate	pKa	H <sub>2</sub> O (DMSO)
ESTERS		
	24.5	(30.3)
	(23.6)	
	(20.0)	
	11	(14.2)
	13	(15.7)
	(20.9)	
	[30.2 (THF)]	
AMIDES		
	(26.6)	
	(25.9)	
	(24.9)	
	(17.2)	
	(18.2)	
	(25.7)	

Substrate	pKa	H <sub>2</sub> O (DMSO)
ETHERS		
CH <sub>3</sub> OPh	(49)	
MeOCH <sub>2</sub> SO <sub>2</sub> Ph	(30.7)	
PhOCH <sub>2</sub> SO <sub>2</sub> Ph	(27.9)	
PhOCH <sub>2</sub> CN	(28.1)	
	(21.1)	
SELENIDES		
	(18.6)	
PhSeCHPh <sub>2</sub>	(27.5)	
(PhSe) <sub>2</sub> CH <sub>2</sub>	(31.3)	
PhSeCH <sub>2</sub> Ph	(31.0)	
PhSeCH=CHCH <sub>2</sub> SePh	(27.2)	
AMMONIUM		
Me <sub>3</sub> N <sup>+</sup> CH <sub>2</sub> X		
X= CN	(20.6)	
SO <sub>2</sub> Ph	(19.4)	
COPh	(14.6)	
CO <sub>2</sub> Et	(20.6)	
CONEt <sub>2</sub>	(24.9)	

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)

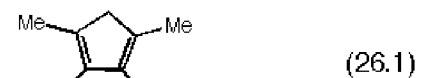
HCCH 24

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>					
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)	DBU	(11-12) (estimate)
SO <sub>2</sub> Ph	(15.1)	CN	(22.0)	DMAP	9.2
	19-20 (27.1)				6.95
	(28.3)	n= 4	(25.1)		
	(27.7)	5	(25.8)	R= H (PPTS)	5.21 (3.4)
	(26.3)	6	(26.4)	<i>t</i> -Bu	4.95 (0.90)
		7	(27.7)	Me	6.75 (4.46)
		8	(27.4)	Cl, H	0.72
X= H	(24.7)		(28.1)	<b>HETEROCYCLES</b>	
CH <sub>3</sub>	(24.4)		(29.0)		(20.95)
Ph	(17.7)		(25.5)		(23.0)
COCH <sub>3</sub>	(12.7)		(25.5)		(18.6)
COPh	(13.3)		(32.4)		
CO <sub>2</sub> Et	(22.7)				(13.9)
CN	(10.2)				
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)

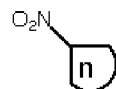
NITRILES		
X= H		(31.3)
CH <sub>3</sub>		(32.5)
Ph		(21.9)
COPh		(10.2)
CONR <sub>2</sub>		(17.1)
CO <sub>2</sub> Et		(13.1)
CN	11	(11.1)
OPh		(28.1)
N <sup>+</sup> Me <sub>3</sub>		(20.6)
SPh		(20.8)
SO <sub>2</sub> Ph		(12.0)

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



(24.3)

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)

PHOSPHONATES & 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
Me <sup>+</sup> OH <sub>2</sub>	-2.2
	-1.8
	0.79

SULFINIC & SULFONIC ACIDS

	-2.6
	7.1

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

SULFIDES

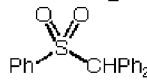
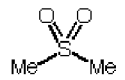
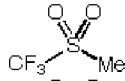
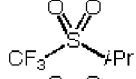

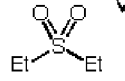
PhSCH <sub>2</sub> X	
X= Ph	(30.8)
CN	(20.8)
COCH <sub>3</sub>	(18.7)
COPh	(16.9)
NO <sub>2</sub>	(11.8)
SPh	(30.8)
SO <sub>2</sub> Ph	(20.3)
SO <sub>2</sub> CF <sub>3</sub>	(11.0)
POPh <sub>2</sub>	(24.9)
MeSCH <sub>2</sub> SO <sub>2</sub> Ph	(23.4)
PhSCHPh <sub>2</sub>	(26.7)
(PhS) <sub>3</sub> CH	(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)  
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 JOC 42, 326 (1977)  
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