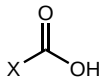
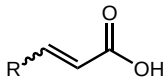
INORGANIC ACIDS

Substrate	pKa H_2O	(DMSO)
H_2O	15.7	(32)
H_3O^+	-1.7	
H_2S	7.00	
HBr	-9.00	(0.9)
HCl	-8.0	(1.8)
HF	3.17	(15)
HOCl	7.5	
$HClO_4$	-10	
HCN	9.4	(12.9)
HN_3	4.72	(7.9)
HSCN	4.00	
H_2SO_3	1.9, 7.21	
H_2SO_4	-3.0, 1.99	
H_3PO_4	2.12, 7.21, 12.32	
HNO_3	-1.3	
HNO_2	3.29	
H_2CrO_4	-0.98, 6.50	
CH_3SO_3H	-2.6	(1.6)
CF_3SO_3H	-14	(0.3)
NH_4Cl	9.24	
$B(OH)_3$	9.23	
HOOH	11.6	

CARBOXYLIC ACIDS



X=	pKa H_2O	(DMSO)
CH_3	4.76	(12.3)
CH_2NO_2	1.68	
CH_2F	2.66	
CH_2Cl	2.86	
CH_2Br	2.86	
CH_2I	3.12	
$CHCl_2$	1.29	
CCl_3	0.65	
CF_3	-0.25	
H	3.77	
HO	3.6, 10.3	
C_6H_5	4.2	(11.1)
o-$O_2NC_6H_4$	2.17	
m-$O_2NC_6H_4$	2.45	
p-$O_2NC_6H_4$	3.44	
o-ClC_6H_4	2.94	
m-ClC_6H_4	3.83	
p-ClC_6H_4	3.99	
o-$(CH_3)_3N^+C_6H_4$	1.37	
p-$(CH_3)_3N^+C_6H_4$	3.43	
p-$OMeC_6H_4$	4.47	

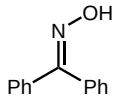


R=	pKa H_2O	(DMSO)
H	4.25	
trans-CO_2H	3.02, 4.38	
cis-CO_2H	1.92, 6.23	

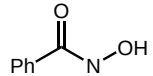
ALCOHOLS

	pKa H_2O	(DMSO)
HOH	15.7	(31.2)
MeOH	15.54	(27.9)
i-PrOH	16.5	(29.3)
t-BuOH	17	(29.4)
c-hex_3COH	24	
CF_3CH_2OH	12.5	(23.5)
$(CF_3)_2CHOH$		(17.9)
C_6H_5OH	9.95	(18.0)
m-$O_2NC_6H_4OH$	8.35	
p-$O_2NC_6H_4OH$	7.14	(10.8)
p-$OMeC_6H_4OH$	10.20	(19.1)
2-napthol		(17.1)

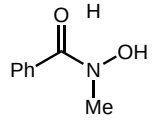
OXIMES & HYDROXAMIC ACIDS



pKa H_2O	(DMSO)
11.3	(20.1)



pKa H_2O	(DMSO)
8.88 (NH)	(13.7)

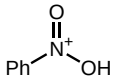


pKa H_2O	(DMSO)
	(18.5)

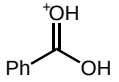
PEROXIDES

	pKa H_2O
MeOOH	11.5
CH_3CO_3H	8.2

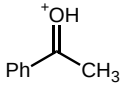
PROTONATED SPECIES



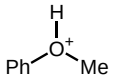
pKa H_2O: -12.4



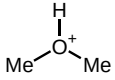
pKa H_2O: -7.8



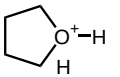
pKa H_2O: -6.2



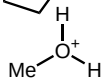
pKa H_2O: -6.5



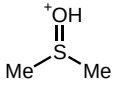
pKa H_2O: -3.8



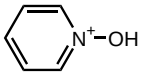
pKa H_2O: -2.05



pKa H_2O: -2.2

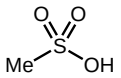


pKa H_2O: -1.8

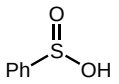


pKa H_2O: 0.79

SULFINIC & SULFONIC ACIDS



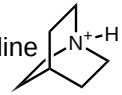
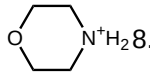
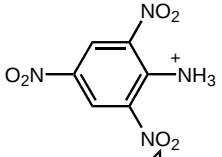
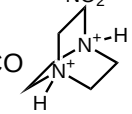
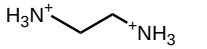
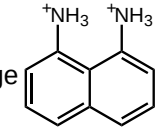
pKa H_2O: -2.6



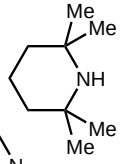
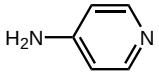
pKa H_2O: 2.1

*Values <0 for H_2O and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

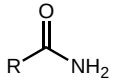
PROTONATED NITROGEN

Substrate	pKa H_2O	(DMSO)
N^+H_4	9.2	(10.5)
EtN^+H_3	10.6	
i-$Pr_2N^+H_2$	11.05	
Et_3N^+H	10.75	(9.00)
PhN^+H_3	4.6	(3.6)
$PhN^+(Me)_2H$	5.20	(2.50)
$Ph_2N^+H_2$	0.78	
2-napthal-N^+H_3	4.16	
$H_2NN^+H_3$	8.12	
HON^+H_3	5.96	
Quinuclidine 	11.0	(9.80)
Morpholine 	8.36	
N-Me morpholine	7.38	
	-9.3	
DABCO 	2.97, 8.82 (2.97, 8.93)	
	6.90, 9.95	
Proton Sponge 	-9.0, 12.0 (--, 7.50)	
$PhCN^+H$	-10	

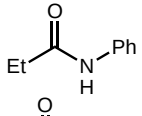
AMINES

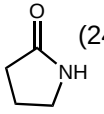
Substrate	pKa H_2O	(DMSO)
HN_3	4.7	(7.9)
NH_3	38	(41)
i-Pr_2NH	(36 THF))	
TMS_2NH	26(THF)	(30)
$PhNH_2$		(30.6)
Ph_2NH		(25.0)
$NCNH_2$		(16.9)
		(44)
TMP 		(37)
		(26.5)

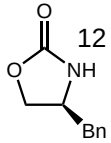
AMIDES & CARBAMATES



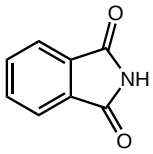
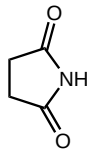
R=			
	H		(23.5)
	CH_3	15.1	(25.5)
	Ph		(23.3)
	CF_3		(17.2)
	NH_2 (urea)		(26.9)
	OEt		(24.8)

 (21.6)

 (24.1)

 12 (20.5)

IMIDES

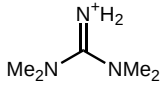
 8.30  (14.7)

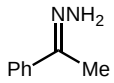
Ac_2NH (17.9)

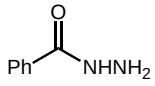
SULFONAMIDE

$MeSO_2NH_2$		(17.5)
$PhSO_2NH_2$		(16.1)
$CF_3SO_2NH_2$	6.3	(9.7)
$MeSO_2NHPh$		(12.9)

GUANIDINIUM, HYRDAZONES,- IDES, & -INES

 (13.6)

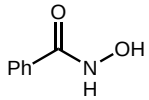
 (21.6)

 (18.9)

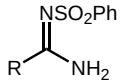
$PhSO_2NHNH_2$ (17.2)

PhNHNHPh (26.1)

HYDROXAMIC ACID

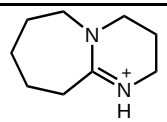
 8.88 (NH) (13.7)

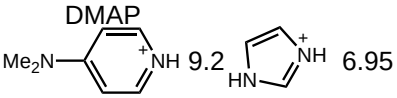
AMIDINES

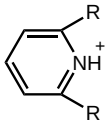


R=		
	Me	(17.3)
	Ph	(15.0)

PROTONATED HETEROCYCLES

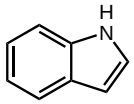
DBU  (12) (estimate)

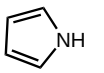
DMAP  9.2 6.95



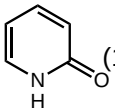
R=			
	H (PPTS)	5.21	(3.4)
	t-Bu	4.95	(0.90)
	Me	6.75	(4.46)
	Cl, H	0.72	

HETEROCYCLES

 (20.95)

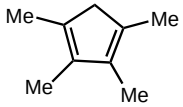
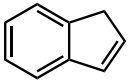
 (23.0)  (18.6)

1,2,3 triazole

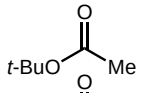
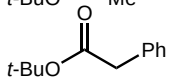
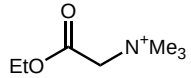
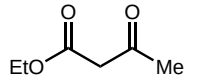
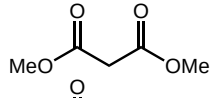
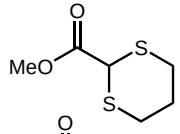
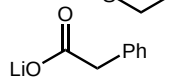
 (17.0)  (13.9)

*Values <0 for H_2O and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

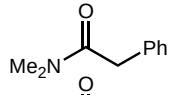
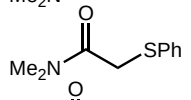
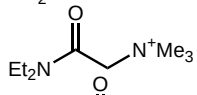
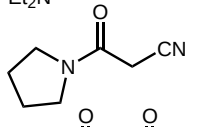
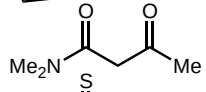
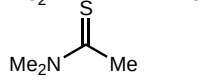
HYDROCARBONS

Substrate	pKa H_2O	(DMSO)
$(Me)_3CH$	53	
$(Me)_2CH_2$	51	
$CH_2{=}CH_2$	50	
CH_4	48	(56)
△	46	
$CH_2{=}CHCH_3$	43	(44)
PhH	43	
$PhCH_3$	41	(43)
Ph_2CH_2	33.5	(32.2)
Ph_3CH	31.5	(30.6)
HCCH	24	
PhCCH	23	(28.8)
$XC_6H_4CH_3$		
X= *p*-CN		(30.8)
p-NO_2		(20.4)
p-COPh		(26.9)
		(26.1)
	20	(20.1)
	15	(18.0)
H_2	~36	

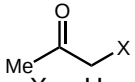
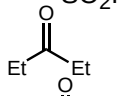
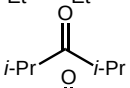
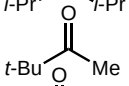
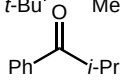
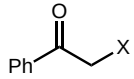
ESTERS

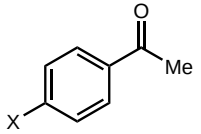
	pKa H_2O	(DMSO)
	24.5	(30.3)
		(23.6)
		(20.0)
	11	(14.2)
	13	(15.7)
		(20.9)
		[30.2 (THF)]

AMIDES

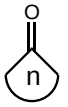
		(26.6)
		(25.9)
		(24.9)
		(17.2)
		(18.2)
		(25.7)

KETONES

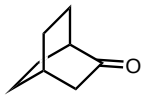
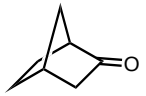
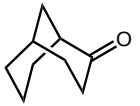
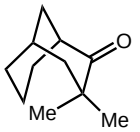
	pKa H_2O	(DMSO)
		
X= H		(26.5)
Ph		(19.8)
SPh		(18.7)
$COCH_3$	9	(13.3)
SO_2Ph		(15.1)
	19-20	(27.1)
		(28.3)
		(27.7)
		(26.3)
		
X= H		(24.7)
CH_3		(24.4)
Ph		(17.7)
$COCH_3$		(12.7)
COPh		(13.3)
CO_2Et		(22.7)
CN		(10.2)
F		(21.6)
OMe		(22.85)
OPh		(21.1)
SPh		(16.9)
SePh		(18.6)
NPh_2		(20.3)
N^+Me_3		(14.6)
NO_2		(7.7)
SO_2Ph		(11.4)



X=	H	(24.7)
	OMe	(25.7)
	NMe_2	(27.5)
	Br	(23.8)
	CN	(22.0)



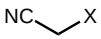
n=	4	(25.1)
	5	(25.8)
	6	(26.4)
	7	(27.7)
	8	(27.4)

	(28.1)
	(29.0)
	(25.5)
	(32.4)

*Values <0 for H_2O and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

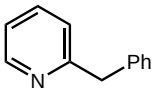
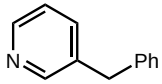
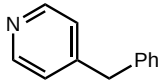
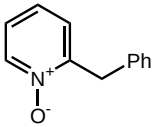
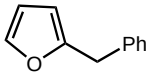
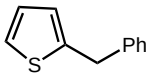
pKa's of CH bonds at Nitrile, Heteroaromatic, and Sulfur Substituted Carbon

NITRILES



X=		pKa H_2O	pKa (DMSO)
	H		(31.3)
	CH_3		(32.5)
	Ph		(21.9)
	COPh		(10.2)
	$CONR_2$		(17.1)
	CO_2Et		(13.1)
	CN	11	(11.1)
	OPh		(28.1)
	N^+Me_3		(20.6)
	SPh		(20.8)
	SO_2Ph		(12.0)

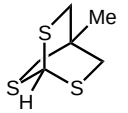
HETERO-AROMATICS

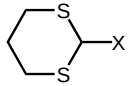
	pKa (DMSO)
	(28.2)
	(30.1)
	(26.7)
	(25.2)
	(30.2)
	(30.0)

SULFIDES

$PhSCH_2X$

X=	pKa (DMSO)
Ph	(30.8)
CN	(20.8)
$COCH_3$	(18.7)
COPh	(16.9)
NO_2	(11.8)
SPh	(30.8)
SO_2Ph	(20.3)
SO_2CF_3	(11.0)
$POPh_2$	(24.9)

	pKa (DMSO)
$MeSCH_2SO_2Ph$	(23.4)
$PhSCHPh_2$	(26.7)
$(PhS)_3CH$	(22.8)
$(PrS)_3CH$	(31.3)
	(30.5)
$(PhS)_2CHPh$	(23.0)



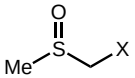
X=	pKa (DMSO)
Ph	(30.7)
CO_2Me	(20.8)
CN	(19.1)

$RSCH_2CN$

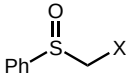
R=	pKa H_2O	pKa (DMSO)
Me		(24.3)
Et		(24.0)
i-Pr		(23.6)
t-Bu		(22.9)

	pKa H_2O	pKa (DMSO)
$PhSCH=CHCH_2SPh$		(26.3)
BuSH	10-11	(17.0)
PhSH	≈7	(10.3)

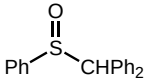
SULFOXIDES



X=	pKa (DMSO)
H	(35.1)
Ph	(29.0)
SPh	(29.0)



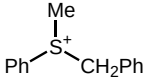
X=	pKa (DMSO)
H	(33)
Ph	(27.2)
SOPh	(18.2)



(24.5)

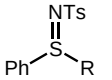
SULFONIUM

	pKa (DMSO)
$Me_3S^+=O$	(18.2)

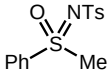


(16.3)

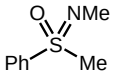
SULFIMIDES & SULFOXIMINES



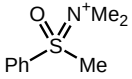
R=	pKa (DMSO)
Me	(27.6)
i-Pr	(30.7)



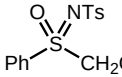
(24.5)



(33)

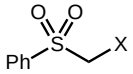


(14.4)

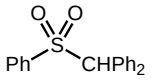
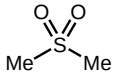
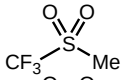
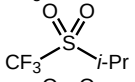
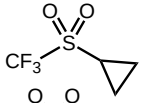
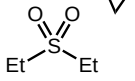


(20.7)

SULFONES

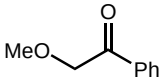
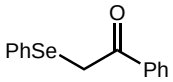


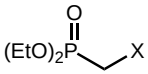
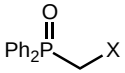
X=	pKa (DMSO)
H	(29.0)
CH_3	(31.0)
t-Bu	(31.2)
Ph	(23.4)
$CH=CH_2$	(22.5)
CH=CHPh	(20.2)
CCH	(22.1)
CCPh	(17.8)
COPh	(11.4)
COMe	(12.5)
OPh	(27.9)
N^+Me_3	(19.4)
CN	(12.0)
NO_2	(7.1)
SMe	(23.5)
SPh	(20.5)
SO_2Ph	(12.2)
PPh_2	(20.2)

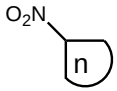
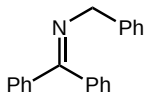
	pKa (DMSO)
	(22.3)
	(31.1)
	(18.8)
	(21.8)
	(26.6)
	(32.8)
$(PhSO_2)_2CH_2Me$	(14.3)

*Values <0 for H_2O and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

pKa's of CH bonds at Heteroatom Substituted Carbon & References

Substrate	pKa H_2O	(DMSO)
ETHERS		
CH_3OPh		(49)
$MeOCH_2SO_2Ph$		(30.7)
$PhOCH_2SO_2Ph$		(27.9)
$PhOCH_2CN$		(28.1)
		(21.1)
SELENIDES		
		(18.6)
$PhSeCHPh_2$		(27.5)
$(PhSe)_2CH_2$		(31.3)
$PhSeCH_2Ph$		(31.0)
$PhSeCH{=}CHCH_2SePh$		(27.2)
AMMONIUM		
$Me_3N^+CH_2X$		
X= CN		(20.6)
SO_2Ph		(19.4)
COPh		(14.6)
CO_2Et		(20.6)
$CONEt_2$		(24.9)

Substrate	pKa H_2O	(DMSO)
PHOSPHONIUM		
P^+H_4		-14
MeP^+H_3		2.7
Et_3P^+H		9.1
$Ph_3P^+CH_3$		(22.4)
$Ph_3P^+i\text{-}Pr$		(21.2)
$Ph_3P^+CH_2COPh$		(6.2)
$Ph_3P^+CH_2CN$		(7.0)
PHOSPONATES & PHOSPHINE OXIDES		
		
X= Ph		(27.6)
CN		(16.4)
CO_2Et		(18.6)
Cl		(26.2)
$SiMe_3$		(28.8)
		
X= SPh		(24.9)
CN		(16.9)
PHOSPHINES		
$Ph_2PCH_2PPh_2$		(29.9)
$Ph_2PCH_2SO_2Ph$		(20.3)

Substrate	pKa H_2O	(DMSO)
NITRO		
RNO_2		
R= CH_3	≈10	(17.2)
CH_2Me		(16.7)
$CHMe_2$		(16.9)
CH_2Ph		(12.2)
CH_2Bn		(16.2)
CH_2SPh		(11.8)
CH_2SO_2Ph		(7.1)
CH_2COPh		(7.7)
		
n= 3		(26.9)
4		(17.8)
5		(16.0)
6		(17.9)
7		(15.8)
IMINES		
		(24.3)

Oxime ethers are ~ 10 pka units less acidic than their ketone counterparts
Streitwieser, JOC 1991, 56, 1989

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*Values <0 for H_2O and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.