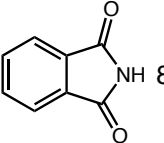
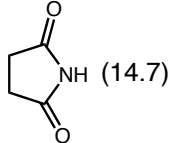
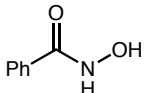
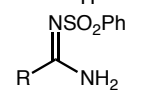
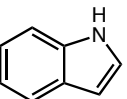
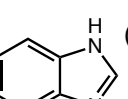
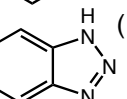
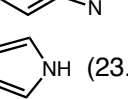
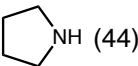
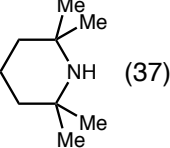
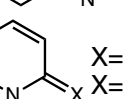
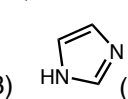
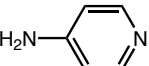
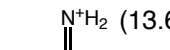
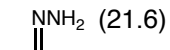
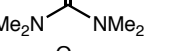
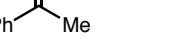
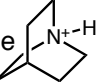
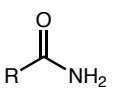
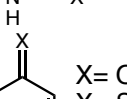
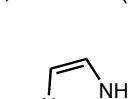
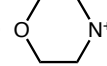
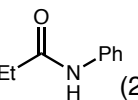
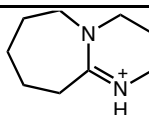
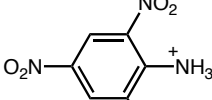
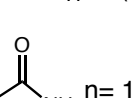
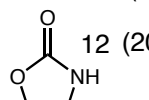
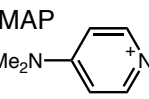
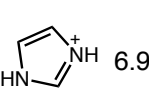
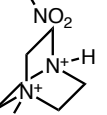
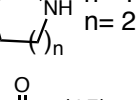
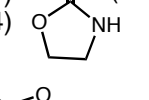
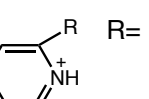
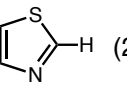
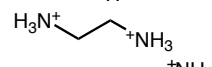
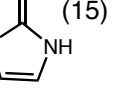
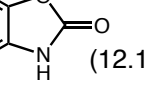
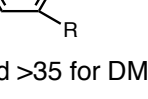
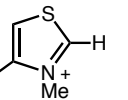
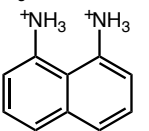
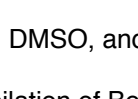
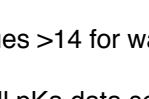
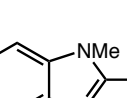
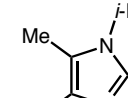


Substrate	pKa	H ₂ O (DMSO)	Substrate	pKa	H ₂ O(DMSO)	Substrate	pKa	H ₂ O (DMSO)	Substrate	pKa	H ₂ O (DMSO)
INORGANIC ACIDS			CARBOXYLIC ACIDS			ALCOHOLS			PROTONATED SPECIES		
H ₂ O	15.7	(32)				HOH	15.7	(31.2)			-12.4
H ₃ O ⁺	-1.7		X= CH ₃	4.76	(12.3)	MeOH	15.5	(27.9)			-7.8
H ₂ S	7.00		CH ₂ NO ₂	1.68		<i>i</i> -PrOH	16.5	(29.3)			-6.2
HBr	-9.00	(0.9)	CH ₂ F	2.66		<i>t</i> -BuOH	17.0	(29.4)			-6.5
HCl	-8.0	(1.8)	CH ₂ Cl	2.86		<i>c</i> -hex ₃ COH	24.0				-3.8
HF	3.17	(15)	CH ₂ Br	2.86		CF ₃ CH ₂ OH	12.5	(23.5)			-2.05
HOCl	7.5		CH ₂ I	3.12		(CF ₃) ₂ CHOH	9.3	(18.2)			-2.2
HClO ₄	-10		CHCl ₂	1.29		C ₆ H ₅ OH	9.95	(18.0)			-1.8
HCN	9.4	(12.9)	CCl ₃	0.65		<i>m</i> -O ₂ NC ₆ H ₄ OH	8.4				0.79 (+1.63)
HN ₃	4.72	(7.9)	CF ₃	-0.25		<i>p</i> -O ₂ NC ₆ H ₄ OH	7.1	(10.8)			(+5.55)
HSCN	4.00		H	3.77		<i>p</i> -OMeC ₆ H ₄ OH	10.2	(19.1)	SULFINIC & SULFONIC ACIDS		
H ₂ SO ₃	1.9, 7.21		HO	3.6, 10.3		2-naphthol		(17.1)			-2.6
H ₂ SO ₄	-3.0, 1.99		C ₆ H ₅	4.2	(11.1)	OXIMES & HYDROXAMIC ACIDS					2.1
H ₃ PO ₄	2.12, 7.21, 12.32		<i>o</i> -O ₂ NC ₆ H ₄	2.17			11.3	(20.1)			
HNO ₃	-1.3		<i>m</i> -O ₂ NC ₆ H ₄	2.45			8.88	(13.7) (NH)			
HNO ₂	3.29		<i>p</i> -O ₂ NC ₆ H ₄	3.44				(18.5)			
H ₂ CrO ₄	-0.98, 6.50		<i>o</i> -ClC ₆ H ₄	2.94		PEROXIDES					
CH ₃ SO ₃ H	-2.6	(1.6)	<i>m</i> -ClC ₆ H ₄	3.83		MeOOH	11.5				
CF ₃ SO ₃ H	-14	(0.3)	<i>p</i> -ClC ₆ H ₄	3.99		CH ₃ CO ₃ H	8.2				
NH ₄ Cl	9.24		<i>o</i> -(CH ₃) ₃ N ⁺ C ₆ H ₄	1.37							
B(OH) ₃	9.23		<i>p</i> -(CH ₃) ₃ N ⁺ C ₆ H ₄	3.43							
HOOH	11.6		<i>p</i> -OMeC ₆ H ₄	4.47							
			R= H	4.25							
			<i>trans</i> -CO ₂ H	3.02, 4.38							
			<i>cis</i> -CO ₂ H	1.92, 6.23							

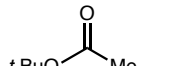
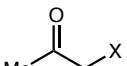
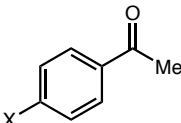
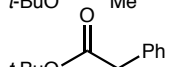
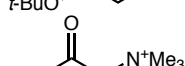
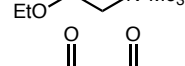

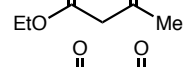
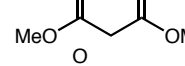
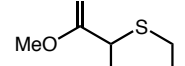
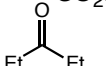

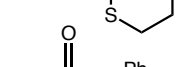
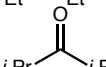
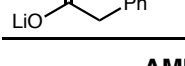
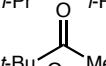
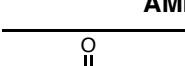
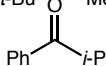
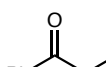
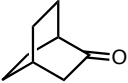
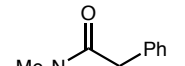
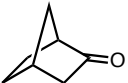
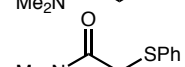
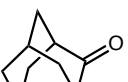
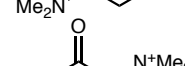

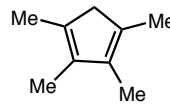
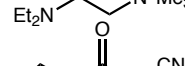
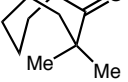
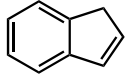
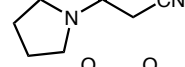

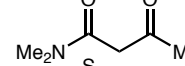
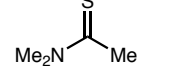
*Values <0 for H₂O and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

For a comprehensive compilation of Bordwell pKa data see: <http://www.chem.wisc.edu/areas/reich/pkatable/index.htm>

Substrate	pKa	H ₂ O (DMSO)	Substrate	pKa	H ₂ O (DMSO)	Substrate	pKa	H ₂ O (DMSO)	Substrate	pKa	H ₂ O (DMSO)			
PROTONATED NITROGEN			AMINES			IMIDES			HYDROXAMIC ACID & AMIDINES					
N ⁺ H ₄	9.2	(10.5)	HN ₃	4.7	(7.9)		8.30			8.88	(13.7)			
EtN ⁺ H ₃	10.6		NH ₃	38	(41)	Ac ₂ NH	(17.9)			R= Me	(17.3)			
<i>i</i> -Pr ₂ N ⁺ H ₂	11.05		<i>i</i> -Pr ₂ NH	(36 THF)					R= Ph	(15.0)				
Et ₃ N ⁺ H	10.75	(9.00)	TMS ₂ NH	26(THF)	(30)	SULFONAMIDE			HETEROCYCLES					
PhN ⁺ H ₃	4.6	(3.6)	PhNH ₂	(30.6)		RSO ₂ NH ₂	R = Me	(17.5)		(20.95)		(16.4)		
PhN ⁺ (Me) ₂ H	5.20	(2.50)	Ph ₂ NH	(25.0)			Ph	(16.1)		(11.9)		(23.0)		
Ph ₂ N ⁺ H ₂	0.78		NCNH ₂	(16.9)		MeSO ₂ NHPh	CF ₃	6.3	(9.7)					
2-naphthal-N ⁺ H ₃	4.16			(44)		(37)				X= O (24)		(18.6)		
H ₂ NN ⁺ H ₃	8.12			(26.5)	AMIDES & CARBAMATES				(13.6)		(21.6)			
HON ⁺ H ₃	5.96					R= H	(23.5)		(18.9)		(17.2)			
Quinuclidine 	11.0	(9.80)		R= CH ₃	15.1	(25.5)	PhSO ₂ NHNH ₂	(17.2)		X= S (13.3)		(13.9)		
Morpholine 	8.36		(urea) NH ₂	(26.9)		PhNHNHPh	(26.1)	PROTONATED HETEROCYCLES						
N-Me morpholine	7.38		OEt	(24.8)		12	(20.5)		(12)	(estimate)				
	-9.3			(21.6)		(20.8)		9.2		6.95				
DABCO 	2.97, 8.82 (2.97, 8.93)			n = 1	(24.1)		(20.8)		R= H (PPTS)	5.21	(3.4)		(29.4)	
	6.90, 9.95			n = 2	(26.4)		(12.1)		<i>t</i> -Bu	4.95	(0.90)		(16.5)	
Proton Sponge 	-9.0, 12.0 (-, 7.50)			(15)		(12.1)		Me	6.75	(4.46)		(18.4)		(24)
PhCN ⁺ H	-10							Cl, H	0.72					

*Values <0 for H₂O and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

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Substrate	pKa	H ₂ O (DMSO)	Substrate	pKa	H ₂ O (DMSO)	Substrate	pKa	H ₂ O (DMSO)	Substrate	pKa	H ₂ O (DMSO)
HYDROCARBONS			ESTERS			KETONES					
(Me) ₃ CH	53			24.5	(30.3)						
(Me) ₂ CH ₂	51				(23.6)	X= H		(26.5)	X= H		(24.7)
CH ₂ =CH ₂	50				(20.0)	Ph		(19.8)	OMe		(25.7)
CH ₄	48	(56)			(20.0)	SPh		(18.7)	NMe ₂		(27.5)
	46			11	(14.2)	COCH ₃	9	(13.3)	Br		(23.8)
CH ₂ =CHCH ₃	43	(44)		13	(15.7)	SO ₂ Ph		(12.5)	CN		(22.0)
PhH	43				(20.9)		19-20	(27.1)			
PhCH ₃	41	(43)			[30.2 (THF)]			(28.3)	n= 4		(25.1)
Ph ₂ CH ₂	33.5	(32.2)						(27.7)	5		(25.8)
Ph ₃ CH	31.5	(30.6)						(26.3)	6		(26.4)
HCCH	24								7		(27.7)
PhCCH	23	(28.8)				X= H		(24.7)	8		(27.4)
XC ₆ H ₄ CH ₃			AMIDES			CH ₃		(24.4)			(28.1)
X= <i>p</i> -CN		(30.8)			(26.6)	Ph		(17.7)			(29.0)
<i>p</i> -NO ₂		(20.4)			(25.9)	COCH ₃		(14.2)			(25.5)
<i>p</i> -COPh		(26.9)			(24.9)	COPh		(13.3)			
		(26.1)			(17.2)	CN		(10.2)			(32.4)
	20	(20.1)			(18.2)	F		(21.6)			
	15	(18.0)			(25.7)	OMe		(22.85)			
H ₂	~36					OPh		(21.1)			
						SPh		(16.9)			
						SePh		(18.6)			
						NPh ₂		(20.3)			
						N ⁺ Me ₃		(14.6)			
						NO ₂		(7.7)			
						SO ₂ Ph		(11.4)			

*Values <0 for H₂O and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

For a comprehensive compilation of Bordwell pKa data see: <http://www.chem.wisc.edu/areas/reich/pkatable/index.htm>

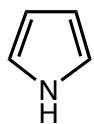
Substrate	pKa	H ₂ O (DMSO)	Substrate	pKa	H ₂ O (DMSO)	Substrate	pKa	H ₂ O (DMSO)	Substrate	pKa	H ₂ O (DMSO)
NITRILES			SULFIDES			SULFOXIDES			SULFONES		
NC-CH ₂ -X			PhSCH ₂ X								
X= H	(31.3)		X= Ph	(30.8)		X= H	(35.1)		X= H	(29.0)	
CH ₃	(32.5)		CN	(20.8)			(29.0)		CH ₃	(31.0)	
Ph	(21.9)		COCH ₃	(18.7)		X= Ph	(29.0)		<i>t</i> -Bu	(31.2)	
COPh	(10.2)		COPh	(16.9)					Ph	(23.4)	
CONR ₂	(17.1)		NO ₂	(11.8)		X= H	(33)		CH=CH ₂	(22.5)	
CO ₂ Et	(13.1)		SPh	(30.8)		Ph	(27.2)		CH=CHPh	(20.2)	
CN	11	(11.1)	SO ₂ Ph	(20.5)		SOPh	(18.2)		CCH	(22.1)	
OPh	(28.1)		SO ₂ CF ₃	(11.0)			(24.5)		CCPh	(17.8)	
N ⁺ Me ₃	(20.6)		POPh ₂	(24.9)		SULFONIUM			COPh	(11.4)	
SPh	(20.8)		MeSCH ₂ SO ₂ Ph	(23.4)		Me ₃ S ⁺ =O	(18.2)		COMe	(12.5)	
SO ₂ Ph	(12.0)		PhSCHPh ₂	(26.7)			(16.3)		OPh	(27.9)	
HETERO-AROMATICS			(PhS) ₃ CH	(22.8)		SULFIMIDES & SULFOXIMINES			N ⁺ Me ₃	(19.4)	
	(28.2)		(PrS) ₃ CH	(31.3)					CN	(12.0)	
	(30.1)			(30.5)		R= Me	(27.6)		NO ₂	(7.1)	
	(26.7)		(PhS) ₂ CHPh	(23.0)		R= <i>i</i> -Pr	(30.7)		SMe	(23.5)	
	(25.2)		X= Ph	(30.7)			(24.5)		SPh	(20.5)	
	(30.2)		CO ₂ Me	(20.8)					SO ₂ Ph	(12.2)	
	(30.0)		CN	(19.1)			(33)		PPh ₂	(20.2)	
			RSCH ₂ CN				(14.4)			(22.3)	
			R= Me	(24.3)			(14.4)			(31.1)	
			Et	(24.0)			(20.7)			(18.8)	
			<i>i</i> -Pr	(23.6)						(21.8)	
			<i>t</i> -Bu	(22.9)						(26.6)	
			PhSCH=CHCH ₂ SPh	(26.3)						(32.8)	
			BuSH	10-11	(17.0)				(PhSO ₂) ₂ CH ₂ Me	(14.3)	
			PhSH	≈7	(10.3)						

*Values <0 for H₂O and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

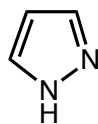
DMSO Acidities of Common Heterocycles

Bordwell, ACR, 1988, 21, 456

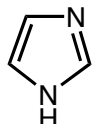
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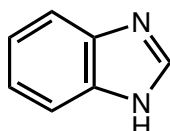
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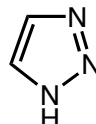
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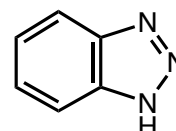
18.6



16.4



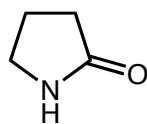
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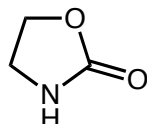
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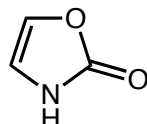
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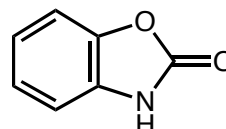
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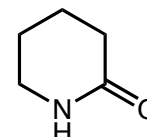
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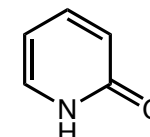
15.0



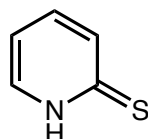
12.1



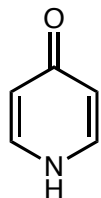
26.4



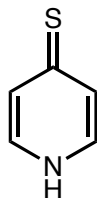
24.0



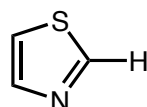
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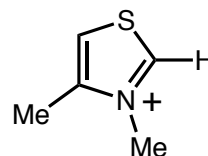
14.8



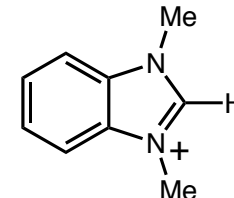
11.8



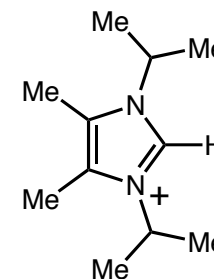
29.4



16.5



18.4



24