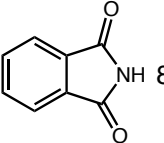
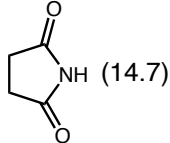
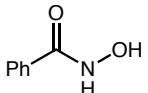
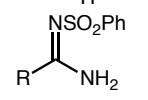
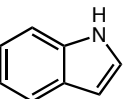
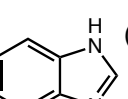
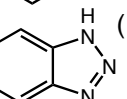
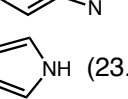
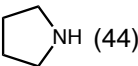
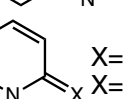
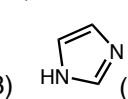
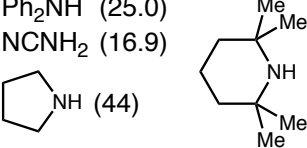
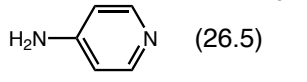
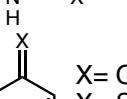
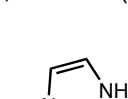
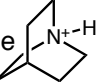
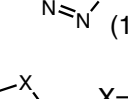
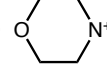
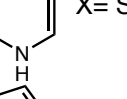
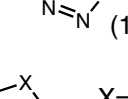
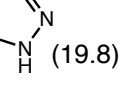
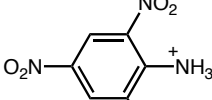
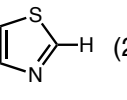
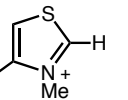
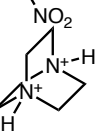
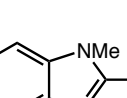
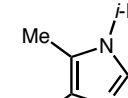
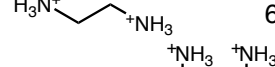
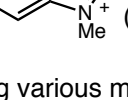
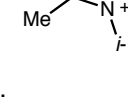
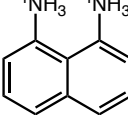
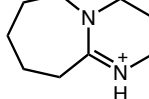
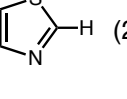
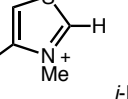
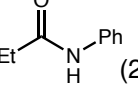
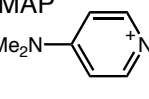
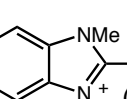
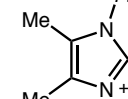
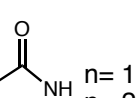
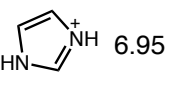
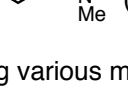
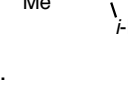
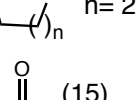
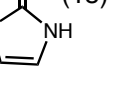
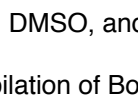



pKa's of Inorganic and Oxo-Acids

Substrate	pKa	H <sub>2</sub> O (DMSO)	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>INORGANIC ACIDS</b>			<b>CARBOXYLIC ACIDS</b>			<b>ALCOHOLS</b>			<b>PROTONATED SPECIES</b>		
H <sub>2</sub> O	15.7	(32)				HOH	15.7	(31.2)			-12.4
H <sub>3</sub> O <sup>+</sup>	-1.7		X= CH <sub>3</sub>	4.76	(12.3)	MeOH	15.5	(27.9)			-7.8
H <sub>2</sub> S	7.00		CH <sub>2</sub> NO <sub>2</sub>	1.68		<i>i</i> -PrOH	16.5	(29.3)			-6.2
HBr	-9.00	(0.9)	CH <sub>2</sub> F	2.66		<i>t</i> -BuOH	17.0	(29.4)			-6.5
HCl	-8.0	(1.8)	CH <sub>2</sub> Cl	2.86		<i>c</i> -hex <sub>3</sub> COH	24.0				-3.8
HF	3.17	(15)	CH <sub>2</sub> Br	2.86		CF <sub>3</sub> CH <sub>2</sub> OH	12.5	(23.5)			-2.05
HOCl	7.5		CH <sub>2</sub> I	3.12		(CF <sub>3</sub> ) <sub>2</sub> CHOH	9.3	(18.2)			-2.2
HClO <sub>4</sub>	-10		CHCl <sub>2</sub>	1.29		C <sub>6</sub> H <sub>5</sub> OH	9.95	(18.0)			-1.8
HCl	-8.0	(1.8)	CCl <sub>3</sub>	0.65		<i>m</i> -O <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> OH	8.4				0.79 (+1.63)
HF	3.17	(15)	CF <sub>3</sub>	-0.25		<i>p</i> -O <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> OH	7.1	(10.8)			(+5.55)
HOCl	7.5		H	3.77		<i>p</i> -OMeC <sub>6</sub> H <sub>4</sub> OH	10.2	(19.1)			
HClO <sub>4</sub>	-10		HO	3.6, 10.3		2-naphthol		(17.1)			
HCl	-8.0	(1.8)	C <sub>6</sub> H <sub>5</sub>	4.2	(11.1)	<b>OXIMES &amp; HYDROXAMIC ACIDS</b>					
HF	3.17	(15)	<i>o</i> -O <sub>2</sub> NC <sub>6</sub> H <sub>4</sub>	2.17			11.3	(20.1)			
HOCl	7.5		<i>m</i> -O <sub>2</sub> NC <sub>6</sub> H <sub>4</sub>	2.45			8.88	(13.7)			
HClO <sub>4</sub>	-10		<i>p</i> -O <sub>2</sub> NC <sub>6</sub> H <sub>4</sub>	3.44			(NH)				
HCl	-8.0	(1.8)	<i>o</i> -ClC <sub>6</sub> H <sub>4</sub>	2.94				(18.5)			
HF	3.17	(15)	<i>m</i> -ClC <sub>6</sub> H <sub>4</sub>	3.83							
HOCl	7.5		<i>p</i> -ClC <sub>6</sub> H <sub>4</sub>	3.99		<b>PEROXIDES</b>					
HClO <sub>4</sub>	-10		<i>o</i> -(CH <sub>3</sub> ) <sub>3</sub> N <sup>+</sup> C <sub>6</sub> H <sub>4</sub>	1.37		MeOOH	11.5				
HCl	-8.0	(1.8)	<i>p</i> -(CH <sub>3</sub> ) <sub>3</sub> N <sup>+</sup> C <sub>6</sub> H <sub>4</sub>	3.43		CH <sub>3</sub> CO <sub>3</sub> H	8.2				
HF	3.17	(15)	<i>p</i> -OMeC <sub>6</sub> H <sub>4</sub>	4.47							
HOCl	7.5										
HClO <sub>4</sub>	-10		R= H	4.25							
HCl	-8.0	(1.8)	<i>trans</i> -CO <sub>2</sub> H	3.02, 4.38							
HF	3.17	(15)	<i>cis</i> -CO <sub>2</sub> H	1.92, 6.23							

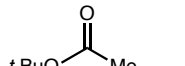
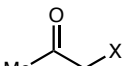
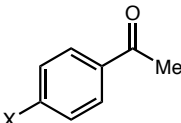
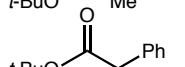
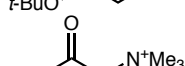
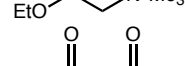

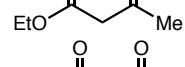
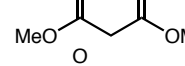
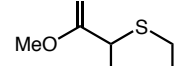
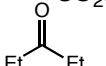

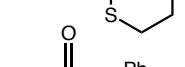
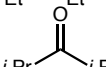
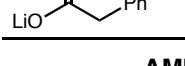
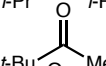
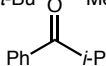
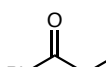
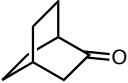
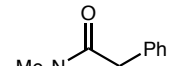
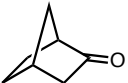
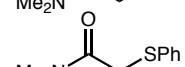
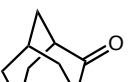
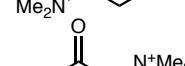
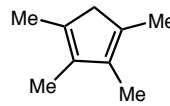
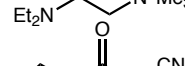
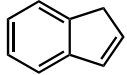
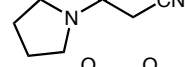

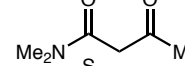
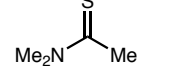
\*Values <0 for H<sub>2</sub>O and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

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

Substrate	pKa	H <sub>2</sub> O	(DMSO)	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>PROTONATED NITROGEN</b>				<b>AMINES</b>				<b>IMIDES</b>				<b>HYDROXAMIC ACID &amp; AMIDINES</b>						
N <sup>+</sup> H <sub>4</sub>	9.2	(10.5)		HN <sub>3</sub>	4.7	(7.9)			8.30									
EtN <sup>+</sup> H <sub>3</sub>	10.6			NH <sub>3</sub>	38	(41)		Ac <sub>2</sub> NH	(17.9)				8.88	(13.7)				
<i>i</i> -Pr <sub>2</sub> N <sup>+</sup> H <sub>2</sub>	11.05			<i>i</i> -Pr <sub>2</sub> NH	(36 THF)								R= Me	(17.3)				
Et <sub>3</sub> N <sup>+</sup> H	10.75	(9.00)		TMS <sub>2</sub> NH	26(THF)	(30)						R= Ph	(15.0)					
PhN <sup>+</sup> H <sub>3</sub>	4.6	(3.6)		PhNH <sub>2</sub>	(30.6)			<b>SULFONAMIDE</b>				<b>HETEROCYCLES</b>						
PhN <sup>+</sup> (Me) <sub>2</sub> H	5.20	(2.50)		Ph <sub>2</sub> NH	(25.0)			RSO <sub>2</sub> NH <sub>2</sub>	R = Me	(17.5)			(20.95)		(16.4)			
Ph <sub>2</sub> N <sup>+</sup> H <sub>2</sub>	0.78			NCNH <sub>2</sub>	(16.9)				Ph	(16.1)			(11.9)		(23.0)			
2-naphthal-N <sup>+</sup> H <sub>3</sub>	4.16				(44)			MeSO <sub>2</sub> NHPh	CF <sub>3</sub>	6.3	(9.7)		X= O (24)		(18.6)			
H <sub>2</sub> NN <sup>+</sup> H <sub>3</sub>	8.12				(37)							X= S (13.3)						
HON <sup>+</sup> H <sub>3</sub>	5.96				(26.5)			<b>GUANIDINIUM, HYDRAZONES, -IDES, &amp; -INES</b>								X= O (14.8)		(13.9)
Quinuclidine 	11.0	(9.80)		<b>AMIDES &amp; CARBAMATES</b>									X= S (11.8)		(13.9)			
Morpholine 	8.36			R= H	(23.5)			Me <sub>2</sub> N=C(NMe <sub>2</sub> ) <sup>+</sup> H <sub>2</sub>	(13.6)				X= O (24)		(18.6)			
N-Me morpholine	7.38			R= CH <sub>3</sub>	15.1	(25.5)		Ph=C(NNH <sub>2</sub> )	(18.9)				X= S (13.3)					
	-9.3			R= Ph	(23.3)			PhSO <sub>2</sub> NHNH <sub>2</sub>	(17.2)				X= O (14.8)		(13.9)			
DABCO 	2.97, 8.82 (2.97, 8.93)			R= CF <sub>3</sub>	(17.2)			PhNHNHPh	(26.1)				X= S (11.8)		(13.9)			
	6.90, 9.95			(urea) NH <sub>2</sub>	(26.9)			<b>PROTONATED HETEROCYCLES</b>								X= O (24.4)		(27.0)
Proton Sponge 	-9.0, 12.0 (-, 7.50)			OEt	(24.8)			DBU 	(12)	(estimate)			(29.4)		(16.5)			
PhCN <sup>+</sup> H	-10				(21.6)			DMAP 	9.2				(16.5)		(24)			
					12	(20.5)			6.95				(18.4)		(24)			
					n = 1	(24.1)		R= H (PPTS)	5.21	(3.4)								
					n = 2	(26.4)		<i>t</i> -Bu	4.95	(0.90)								
								Me	6.75	(4.46)								
								Cl, H	0.72									

\*Values <0 for H<sub>2</sub>O 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>

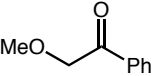
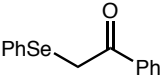
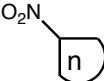
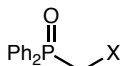
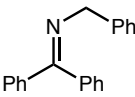
Substrate	pKa	H <sub>2</sub> O (DMSO)	Substrate	pKa	H <sub>2</sub> O (DMSO)	Substrate	pKa	H <sub>2</sub> O (DMSO)	Substrate	pKa	H <sub>2</sub> O (DMSO)
<b>HYDROCARBONS</b>			<b>ESTERS</b>			<b>KETONES</b>					
(Me) <sub>3</sub> CH	53			24.5	(30.3)						
(Me) <sub>2</sub> CH <sub>2</sub>	51				(23.6)	X= H		(26.5)	X= H		(24.7)
CH <sub>2</sub> =CH <sub>2</sub>	50				(20.0)	Ph		(19.8)	OMe		(25.7)
CH <sub>4</sub>	48	(56)			(20.0)	SPh		(18.7)	NMe <sub>2</sub>		(27.5)
	46			11	(14.2)	COCH <sub>3</sub>	9	(13.3)	Br		(23.8)
CH <sub>2</sub> =CHCH <sub>3</sub>	43	(44)		13	(15.7)	SO <sub>2</sub> Ph		(12.5)	CN		(22.0)
PhH	43				(15.7)		19-20	(27.1)			
PhCH <sub>3</sub>	41	(43)			(20.9)			(28.3)	n= 4		(25.1)
Ph <sub>2</sub> CH <sub>2</sub>	33.5	(32.2)			[30.2 (THF)]			(27.7)	5		(25.8)
Ph <sub>3</sub> 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 <sub>6</sub> H <sub>4</sub> CH <sub>3</sub>			<b>AMIDES</b>			CH <sub>3</sub>		(24.4)			(28.1)
X= <i>p</i> -CN		(30.8)			(26.6)	Ph		(17.7)			(29.0)
<i>p</i> -NO <sub>2</sub>		(20.4)			(25.9)	COCH <sub>3</sub>		(14.2)			(25.5)
<i>p</i> -COPh		(26.9)			(24.9)	COPh		(13.3)			
		(26.1)			(17.2)	CN		(10.2)			
	20	(20.1)			(18.2)	F		(21.6)			
	15	(18.0)			(25.7)	OMe		(22.85)			
H <sub>2</sub>	~36					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)			

\*Values <0 for H<sub>2</sub>O 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 <sub>2</sub> O (DMSO)	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>NITRILES</b>			<b>SULFIDES</b>			<b>SULFOXIDES</b>			<b>SULFONES</b>		
NC-CH <sub>2</sub> -X			PhSCH <sub>2</sub> X								
X= H	(31.3)		X= Ph	(30.8)		X= H	(35.1)		X= H	(29.0)	
CH <sub>3</sub>	(32.5)		CN	(20.8)			(29.0)		CH <sub>3</sub>	(31.0)	
Ph	(21.9)		COCH <sub>3</sub>	(18.7)		X= Ph	(29.0)		<i>t</i> -Bu	(31.2)	
COPh	(10.2)		COPh	(16.9)					Ph	(23.4)	
CONR <sub>2</sub>	(17.1)		NO <sub>2</sub>	(11.8)		X= H	(33)		CH=CH <sub>2</sub>	(22.5)	
CO <sub>2</sub> Et	(13.1)		SPh	(30.8)		Ph	(27.2)		CH=CHPh	(20.2)	
CN	11	(11.1)	SO <sub>2</sub> Ph	(20.5)		SOPh	(18.2)		CCH	(22.1)	
OPh	(28.1)		SO <sub>2</sub> CF <sub>3</sub>	(11.0)			(24.5)		CCPh	(17.8)	
N <sup>+</sup> Me <sub>3</sub>	(20.6)		POPh <sub>2</sub>	(24.9)		<b>SULFONIUM</b>			COPh	(11.4)	
SPh	(20.8)		MeSCH <sub>2</sub> SO <sub>2</sub> Ph	(23.4)		Me <sub>3</sub> S <sup>+</sup> =O	(18.2)		COMe	(12.5)	
SO <sub>2</sub> Ph	(12.0)		PhSCHPh <sub>2</sub>	(26.7)			(16.3)		OPh	(27.9)	
<b>HETERO-AROMATICS</b>			(PhS) <sub>3</sub> CH	(22.8)		<b>SULFIMIDES &amp; SULFOXIMINES</b>			N <sup>+</sup> Me <sub>3</sub>	(19.4)	
	(28.2)		(PrS) <sub>3</sub> CH	(31.3)					CN	(12.0)	
	(30.1)			(23.0)			(33)		NO <sub>2</sub>	(7.1)	
	(26.7)			(23.0)			(14.4)		SMe	(23.5)	
	(25.2)		X= Ph	(30.7)			(14.4)		SPh	(20.5)	
	(30.2)		CO <sub>2</sub> Me	(20.8)			(20.7)		SO <sub>2</sub> Ph	(12.2)	
	(30.0)		CN	(19.1)					PPh <sub>2</sub>	(20.2)	
			RSCH <sub>2</sub> CN							(22.3)	
			R= Me	(24.3)						(31.1)	
			Et	(24.0)						(18.8)	
			<i>i</i> -Pr	(23.6)						(21.8)	
			<i>t</i> -Bu	(22.9)						(26.6)	
			PhSCH=CHCH <sub>2</sub> SPh	(26.3)						(32.8)	
			BuSH	10-11	(17.0)				(PhSO <sub>2</sub> ) <sub>2</sub> CH <sub>2</sub> Me	(14.3)	
			PhSH	≈7	(10.3)						

\*Values <0 for H<sub>2</sub>O and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

Substrate	pKa	H <sub>2</sub> O (DMSO)	Substrate	pKa	H <sub>2</sub> O (DMSO)	Substrate	pKa	H <sub>2</sub> O (DMSO)	REFERENCES
<b>ETHERS</b>			<b>PHOSPHONIUM</b>			<b>NITRO</b>			DMSO: JACS <u>97</u> , 7007 (1975) JACS <u>97</u> , 7160 (1975) JACS <u>97</u> , 442 (1975) JACS <u>105</u> , 6188 (1983) JOC <u>41</u> , 1883 (1976) JOC <u>41</u> , 1885 (1976) JOC <u>41</u> , 2786 (1976) JOC <u>41</u> , 2508 (1976) JOC <u>42</u> , 1817 (1977) JOC <u>42</u> , 321 (1977) JOC <u>42</u> , 326 (1977) JOC <u>43</u> , 3113 (1978) JOC <u>43</u> , 3095 (1978) JOC <u>43</u> , 1764 (1978) JOC <u>45</u> , 3325 (1980) JOC <u>45</u> , 3305 (1980) JOC <u>45</u> , 3884 (1980) JOC <u>46</u> , 4327 (1981) JOC <u>46</u> , 632 (1981) JOC <u>47</u> , 3224 (1982) JOC <u>47</u> , 2504 (1982) Acc. Chem. Res. <u>21</u> , 456 (1988) Unpublished results of F. Bordwell
CH <sub>3</sub> OPh	(49)		P <sup>+</sup> H <sub>4</sub>	-14		RNO <sub>2</sub>			
MeOCH <sub>2</sub> SO <sub>2</sub> Ph	(30.7)		MeP <sup>+</sup> H <sub>3</sub>	2.7		R= CH <sub>3</sub>	≈10	(17.2)	
PhOCH <sub>2</sub> SO <sub>2</sub> Ph	(27.9)		Et <sub>3</sub> P <sup>+</sup> H	9.1		CH <sub>2</sub> Me		(16.7)	
PhOCH <sub>2</sub> CN	(28.1)		Ph <sub>3</sub> P <sup>+</sup> CH <sub>3</sub>	(22.4)		CHMe <sub>2</sub>		(16.9)	
	(22.85)		Ph <sub>3</sub> P <sup>+</sup> <i>i</i> -Pr	(21.2)		CH <sub>2</sub> Ph		(12.2)	
<b>SELENIDES</b>			Ph <sub>3</sub> P <sup>+</sup> CH <sub>2</sub> COPh	(6.2)		CH <sub>2</sub> Bn		(16.2)	
	(18.6)		Ph <sub>3</sub> P <sup>+</sup> CH <sub>2</sub> CN	(7.0)		CH <sub>2</sub> SPh		(11.8)	
PhSeCHPh <sub>2</sub>	(27.5)		<b>PHOSPHONATES &amp; PHOSPHINE OXIDES</b>						
(PhSe) <sub>2</sub> CH <sub>2</sub>	(31.3)		(EtO) <sub>2</sub> P(=O)CH <sub>2</sub> X			n= 3		(26.9)	
PhSeCH <sub>2</sub> Ph	(31.0)		X= Ph	(27.6)		4		(17.8)	
PhSeCH=CHCH <sub>2</sub> SePh	(27.2)		CN	(16.4)		5		(16.0)	
<b>AMMONIUM</b>			CO <sub>2</sub> Et	(18.6)		6		(17.9)	
Me <sub>3</sub> N <sup>+</sup> CH <sub>2</sub> X			Cl	(26.2)		7		(15.8)	
X= CN	(20.6)		SiMe <sub>3</sub>	(28.8)		<b>IMINES</b>			
SO <sub>2</sub> Ph	(19.4)							(24.3)	
COPh	(14.6)		X= SPh	(24.9)		Oxime ethers are ~ 10 pka units less acidic than their ketone counterparts Streitwieser, JOC 1991, 56, 1989			
CO <sub>2</sub> Et	(20.0)		CN	(16.9)		Water: Advanced Org. Chem., 3rd Ed. J. March (1985) Unpublished results of W. P. Jencks			
CONEt <sub>2</sub>	(24.9)		<b>PHOSPHINES</b>			THF: JACS <u>110</u> , 5705 (1988)			
			Ph <sub>2</sub> PCH <sub>2</sub> PPh <sub>2</sub>	(29.9)		See cited website below for additional data			
			Ph <sub>2</sub> PCH <sub>2</sub> SO <sub>2</sub> Ph	(20.2)					

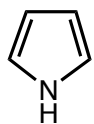
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For a comprehensive compilation of Bordwell pKa data see: <http://www.chem.wisc.edu/areas/reich/pkatable/index.htm>

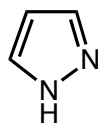
## DMSO Acidities of Common Heterocycles

Bordwell, ACR, 1988, 21, 456

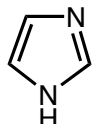
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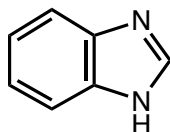
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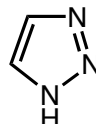
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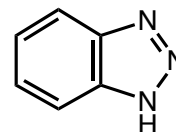
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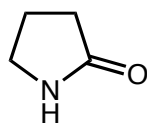
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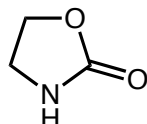
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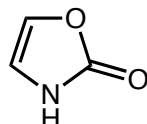
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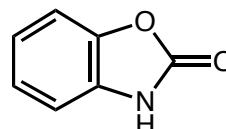
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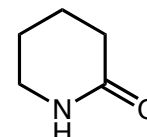
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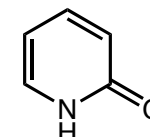
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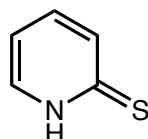
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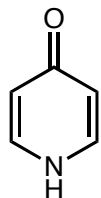
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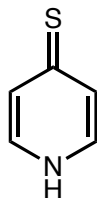
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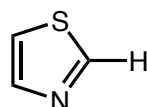
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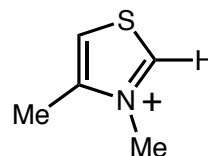
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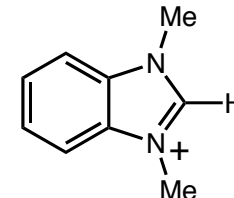
11.8



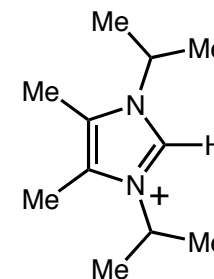
29.4



16.5



18.4



24