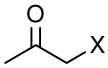
Author: Prof. Hans Reich

Updated 4/11/2022

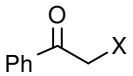
Equilibrium pKa Table (DMSO Solvent and Reference)

Ketones

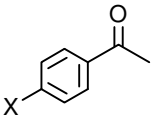


X =	pKa
H	26.5[52]
Ph	19.8[58]
OMe	24.6[27]
SPh	18.7
$COCH_3$	13.3
S(O)Ph	15.1
SO_2Ph	12.5[58]
$^+NMe_3$	16.3[44]
^+Py	11.8[44]

Ar =	pKa
Ph	24.7[1]
2-Py	23.6
4-Py	21.8
2-Furyl	23.9
2-Thienyl	24.0

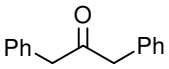


X =	pKa
H	24.7[52]
Me	24.4[58]
Ph	17.7[58]
COMe	14.2[58]
COPh	13.4[42]
C≡N	10.2[6]
F	21.7[52]
OPh	21.1[34]
OMe	22.9[34]
NPh_2	20.3
NMe_2	23.6[57]
$^+NMe_3$	14.6[6]
^+Py	10.7[44]
NO_2	7.7[6]
SPh	17.1[35]
SO_2Ph	11.4[6]
SePh	18.6[5]

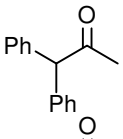


X =	pKa
H	24.7[1]
p-Me	25.2
p-Ph	24.5
p-OMe	25.7[50]
m-OMe	24.5[50]
p-NMe_2	27.5[50]
m-NMe_2	25.3[50]
p-F	24.5[50]
m-F	23.5[50]
p-Cl	23.8[50]
m-Cl	23.2[50]
p-Br	23.8[50]
p-SPh	23.8[50]
p-S(O)Ph	23.2
p-SO_2Ph	22.1[50]
m-SO_2Ph	23.0[50]
p-C≡N	22.0[50]
p-CF_3	22.7[50]
m-CF_3	22.8[50]

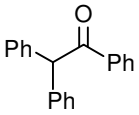
Ketones



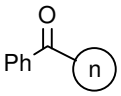
18.7[58]



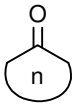
19.4[58]



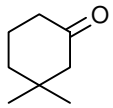
18.8[58]



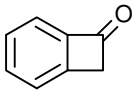
n	pKa
3	28.2
4	24.9
5	25.8
6	26.7[58]
7	27.7
8	27.4



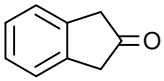
n	pKa
4	26.2
5	25.8[51]
6	26.4[51]
7	27.8
8	27.4
10	26.7
12	26.9



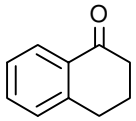
24.8[59]



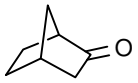
25.8



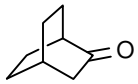
16.9[51]



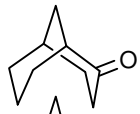
24.7



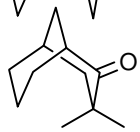
29.0



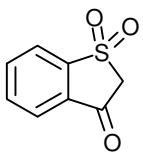
28.1



25.5

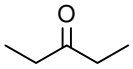


32.4

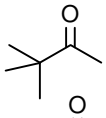


10.1[53]

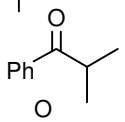
Ketones



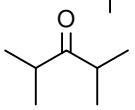
27.1[1]



27.7[58]

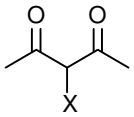


26.3[58]

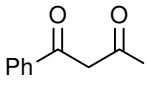


28.2[58]

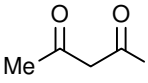
β-Diketones



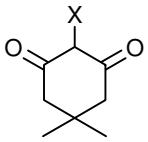
X =	pKa
H	13.3[42]
Me	15.1[42]
Et	15.3[43]
Ac	8.6[43]



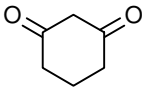
13.4[42]



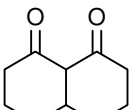
14.2[58]



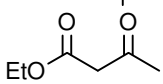
X =	pKa
H	11.2[42]
Me	11.3[43]
Ac	9.8[43]



10.3[59]

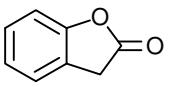


18.2[42]

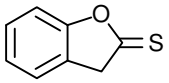


14.2[52]

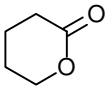
Lactones



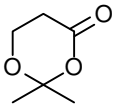
13.5[51]



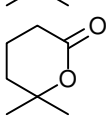
10.7[51]



25.2[59]

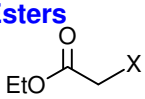


23.3[59]

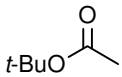


24.5[59]

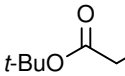
Esters



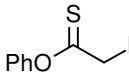
X =	pKa
H	29.5[44]
$^+NMe_3$	20.0[44]
^+Py	14.1[44]
Ph	22.7[18]
CN	13.1[18]
(MeO) SPh	21.4[52]
SO_2CF_3	6.4[61]
NO_2	9.1[61]



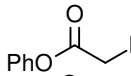
30.3



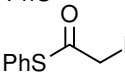
23.6[18]



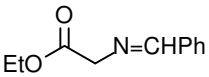
16.9[51]



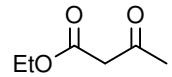
18.7[51]



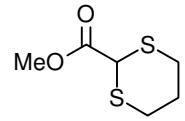
16.9[51]



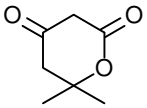
19.5[38]



14.2[58]

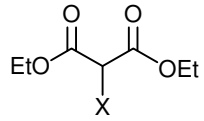


20.9

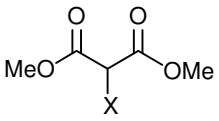


11.5[59]

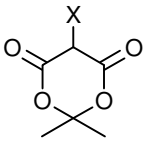
Malonate Esters



X =	pKa
H	16.4[42]
$^+NMe_3$	11.8[44]
^+Py	5.6[44]



X =	pKa
H	15.9[43]
Me	18.0[43]
Et	18.5[43]
CO_2Me	10.8[43]
CF_3	10.8



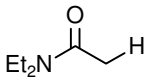
X =	pKa
H	7.3[43]
Me	7.4[43]
Et	7.6[43]

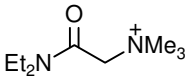
Author: Prof. Hans Reich

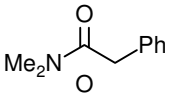
Updated 4/11/2022

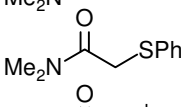
Equilibrium pKa Table (DMSO Solvent and Reference)

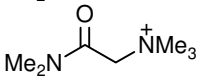
Amides (C-H)

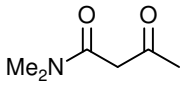

(35)

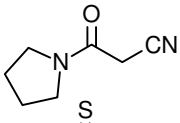

24.9[44]

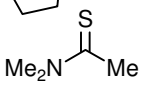

26.6[18]

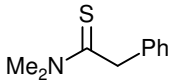

25.9[18]

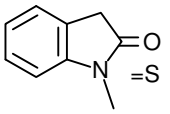

24.9[18]

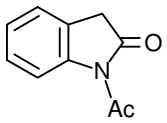

18.2[51]


17.2[18]

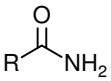

25.7[51]


21.3[51]

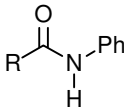

18.5[51]
10.0[51]


13.5[51]

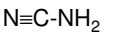
Amides (NH)

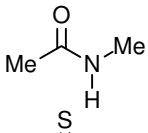


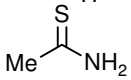
R =		
	H	23.5[13]
	Me	25.5[13]
	CH_2OPh	23.0[27]
	CH_2OMe	23.9[27]
	CH_2SPh	23.0[27]
	CH_2F	22.3[27]
	CH_2NH_2	24.7
	$CH_2NMe_3^+$	15.3[27]
	Ph	23.3[41]
	3-Py	22.0[27]
	4-Py	21.6[27]
	2-Fu	22.5
	CF_3	17.2[52]
	OEt	24.2[51]
	NH_2	26.9

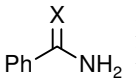


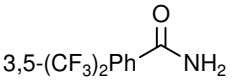
R =		
	Me	21.5[41]
	Ph	18.8[41]
	CH_2F	18.2
	CH_2OMe	19.4
	CH_2SPh	19.0
	CF_3	12.6

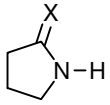

17.0[57]

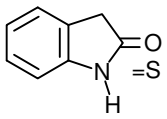

25.9[57]

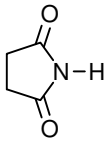

18.5[41]

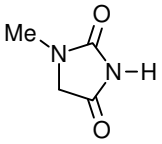

X = O 23.3
X = S 16.9[41]


16.9[41]

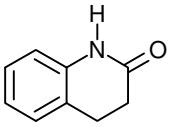

X = O 24.2[51]
X = S 13.3

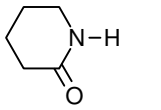

18.5[51]
10.0[51]

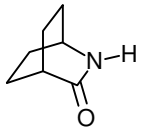

14.7

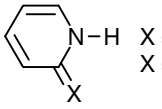

15.0[48]

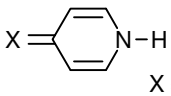
Amides (NH)

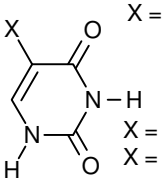

20.7[51]


26.6[51]

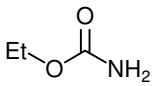

25.4

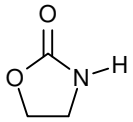

X = O 17.0
X = S 13.3


X = O 14.8
X = S 11.9


X = H 14.1
X = F 12.7

Carbamates (NH)

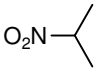

24.2[51]

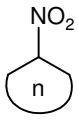

20.8[51]

Nitro

$O_2N\text{-}CH_2\text{-}X$

X =		
	H	17.2[1]
	Me	16.7[1]
	Et	17.0
	Ph	12.2[9]
	SPh	11.8[10]
	SO_2Ph	7.1[6]
	COPh	7.7[6]
	$CH=CH_2$	11.3


16.9[2]

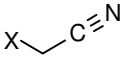


n =		
	3	26.9[12]
	4	17.8[12]
	5	16.0[12]
	6	17.9[12]
	7	15.8[12]

Acetylenes

Ph-C≡C-H 28.8[1,23]

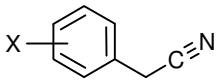
Nitriles



X =		
	H	31.3[1]
	Me	32.5[5]
	Ph	21.9[9]
	C_6F_5	15.8[37]
	2-Furyl	21.4
	1-Naphthyl	20.9[60]
	2-Naphthyl	20.7[60]
	9-Anthryl	19.8[60]
	COPh	10.2[6]

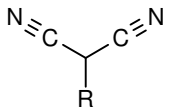

17.2[18]

	CO_2Et	13.1[18]
	C≡N	11.1[1]
	OPh	28.1[5]
	$^+NMe_3$	20.6[6]
	^+Py	16.5[44]
	SPh	20.8[5]
	SMe	24.3[36]
	SO_2Ph	12.0[6]



X =		
	H	21.9[9,60]
	p-Me	22.9[60]
	Me_3	24.6
	p-Ph	20.8[60]
	p-Bz	16.0[60]
	p-NMe_2	24.6[60]
	p-OMe	23.8[60]
	m-OMe	21.6[60]
	p-F	22.2[37,60]
	m-F	20.0[37,60]
	o-F	20.4[37]
	p-Cl	20.5[60]
	m-Cl	19.5[60]
	m-Br	19.4[60]
	p-CN	16.0[60]
	m-CN	18.7[60]
	p-NO_2	12.3[60]
	m-NO_2	18.1[60]
	m-CF_3	19.2[60]
	p-SPh	19.6[60]
	m-SPh	20.4[60]
	p-SO_2Ph	15.8[60]
	m-SO_2Ph	18.5[60]
$(NC)_2CHCH_3$		12.4[13]
$N≡CCHPh_2$		17.5[9,60]
$N≡CCH(C_6F_5)_2$		8.0[37]
N≡C-Fl		8.3[1]
PhCH(Me)CN		23.0[60]

Malononitriles



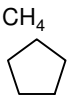
R =		
	H	11.1[1]
	Me	12.4[13]
	Ph	4.2
	$pClC_6H_4$	3.1
	$pMeOC_6H_4$	5.6
	tBu	13.2
	NH_2	13.7[34]
	NMe_2	

Author: Prof. Hans Reich

Updated 4/11/2022

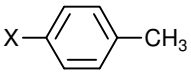
Equilibrium pKa Table (DMSO Solvent and Reference)

Hydrocarbons

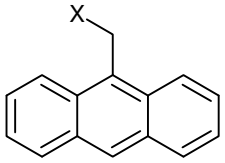


CH_4 (~56)[52]

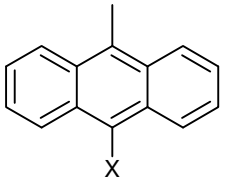
(~59)[19]



X =		
	H	(~43)[11]
	C≡N	30.8[11]
	NO_2	20.4[11]
	$^{+}NMe_3$	31.9[44]
	^{+}Py	20.5[44]
	COPh	26.9[11]
	SO_2Ph	29.8[11]
	SO_2CF_3	24.0[11]



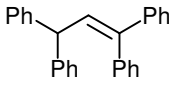
X =		
	H	31.1
	OMe	30.6
	OPh	30.2
	SHex	29.9
	SPh	28.6
	CH_3	32.4
	CN	19.7
	NO_2	12.7



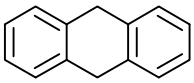
X =		
	H	31.1
	CH_3	31.8
	Cl	28.2
	Br	28.4
	CN	20.0
	NO_2	13.2

Ph_2CH_2	32.3[3]
$(CH_2{=}CH)_2CH_2$	35.[19]
$(C_6F_5)_2CH_2$	22.0[37]
$(p\text{-}O_2N\text{-}C_6H_4)_2CH_2$	15.2[54]
Ph_3CH	30.6[1]
$(p\text{-}Cl\text{-}C_6H_4)_3CH$	27.0
$(p\text{-}O_2N\text{-}C_6H_4)_3CH$	12.7[54]

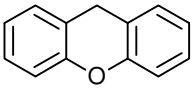
Hydrocarbons



25.8

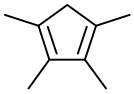


30.1[9]

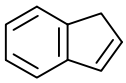


30.0[9]

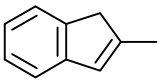
18.0[19]



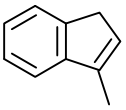
26.1[22]



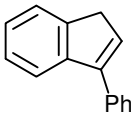
20.1[17]



21.8[22]

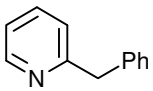


22.5[22]

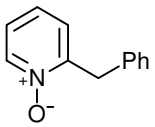


17.3[17]

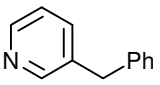
Heteroaromatics



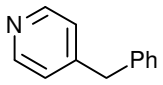
28.2



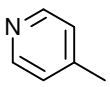
25.2



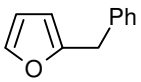
30.1



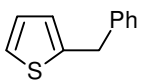
26.7



(35)[52]

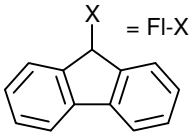


30.2



30.0

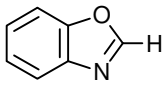
Fluorenes



X = Fl-X

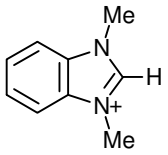
X =		
	H	22.6[1]
	Me	22.3[1]
	Et	22.3[21]
	Pr	22.2
	^{i}Pr	23.2[21]
	^{t}Bu	24.4[21]
	i-Bu	21.6
	$CH_2{}^{t}Bu$	20.3
	Ph	17.9[1]
	o-Tol	18.8
	p-Tol	18.3
	C_6F_5	14.8
	CH_2OH	23.2
	$SiMe_3$	21.5[26]
	$SiPh_3$	18.6[26]
	C(O)Ph	10.0
	CO_2Me	10.3[1]
	C(O)SEt	8.8
	$C(O)NH_2$	14.8
	CN	8.3[1]
	NC	12.3[52]
	NO_2	7.1
	NH_2	22.1[34]
	NMe_2	22.5[34]
	$+NMe_3$	17.8[33]
	^{+}Py	11.8[44]
	$^{+}PPh_3$	6.6[33]
	OMe	22.1[5]
	$O^{i}Pr$	21.4[5]
	OtBu	21.3[5]
	OPh	19.9[5]
	SMe	18.0[7]
	$S^{i}Pr$	16.9
	$S^{t}Bu$	15.9
	SPh	15.5[5]
	S(O)Ph	15.1
	S(O)Bn	15.7
	$S(O_2)Me$	12.8
	$S(O_2)Et$	12.3
	$S(O_2){}^{t}Bu$	12.3
	$S(O_2)Ph$	11.5
	F	22.3
	Cl	18.9

Oxazole

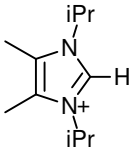


24.4[52]

Imidazolium

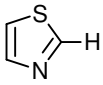


18.6[52]

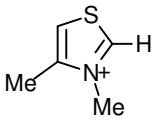


24.[49]

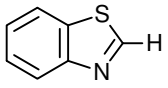
Thiazole



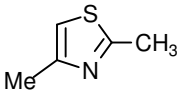
29.4[52]



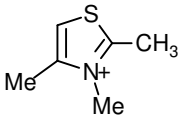
16.5[30]



27.0[52]



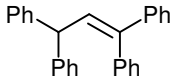
30.3[52]



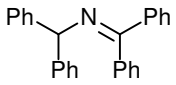
13.9[40]

Allyl

$CH_2{=}CH\text{-}CH_3$	(44)[52]
$(CH_2{=}CH)_2CH_2$	35.[19]

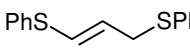


25.8[52]

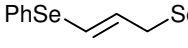


26.5

$Ph_3\overset{+}{P}\text{-}CH_2\text{-}CH{=}CH_2$	18.5[29]
$Ph_3\overset{+}{P}\text{-}CH_2\text{-}CH{=}CHPh$	15.6[29]

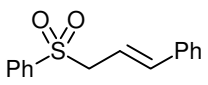


26.3



26.3

$PhSO_2\text{-}CH_2CH{=}CH_2$	22.5[52]
$O_2N\text{-}CH_2CH{=}CH_2$	11.3



20.2[51]

Propargyl

$PhSO_2\text{-}CH_2C{\equiv}CH$	22.1
$PhSO_2\text{-}CH_2C{\equiv}CPh$	17.8

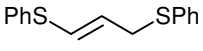
Author: Prof. Hans Reich

Updated 4/11/2022

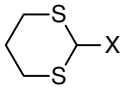
Equilibrium pKa Table (DMSO Solvent and Reference)

Sulfides

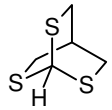
$MeS-CH_3$	(45)[52]
$PhS-CH_2-X$	
X = H	(42)[52]
Ph	30.8[10]
C≡N	20.8[5]
COMe	18.7[10]
COPh	17.1[35]
NO_2	11.8[10]
$^+NMe_3$	28.0[44]
^+Py	17.7[44]
SPh	30.8[3]
SO_2Ph	20.5[5]
SO_2CF_3	11.0[10]
$POPh_2$	24.9
$MeS-CH_2-SO_2Ph$	23.4[5]
MeS-Fl	18.0[7]
PhS-Fl	15.5[5]
$MeS-CH_2-CN$	24.3[21]
t-$BuS-CH_2-CN$	22.9[21]
$PhSCHPh_2$	26.7[10]
$(PhS)_2CHPh$	23.0[10]



26.3

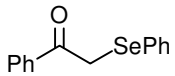


X = H	(39)[23]
Ph	30.7[10]
PhPh	29.0[23]
CO_2Me	20.8[23]
C≡N	19.1[23]
$(PhS)_3CH$	22.8[10]
$(PrS)_3CH$	31.3[52]



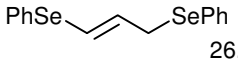
30.5[10]

Selenides



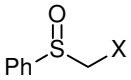
18.6[5]

$PhSeCHPh_2$	27.5
$(PhSe)_2CH_2$	31.3
$PhSeCH_2Ph$	31.0
$(PhSe)_2CHPh$	16.2[52]

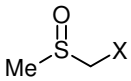


26.3

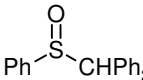
Sulfoxides



X = H	33.[15]
Ph	27.2
SOPh	18.2

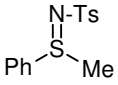


X = H	35.1[1]
SMe	29.0
Ph	29.0[1]

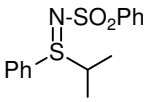


24.6

Sulfimides

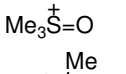


27.6

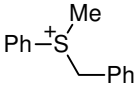


30.7

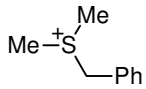
Sulfonium Salts



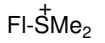
18.2



16.3

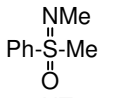


17.8[32]

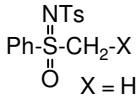


6.5[32]

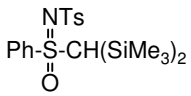
Sulfoximides (C-H)



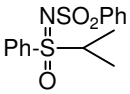
33.0[15]



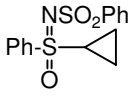
X = H	24.5[15]
Cl	20.7



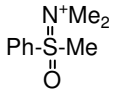
19.1[26]



28.5

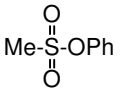


28.7

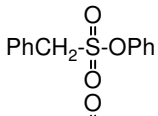


14.4[15]

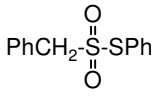
Sulfonates



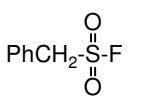
25.2



19.9[53]

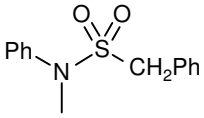


19.1



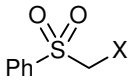
16.9

Sulfonamides (C-H)

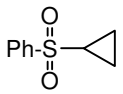


24.1[53]

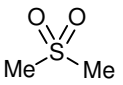
Sulfones



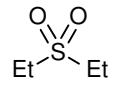
X = H	29.0[1]
Me	31.0[5]
t-Bu	31.2[5]
Ph	23.4[1]
α-Naphth	22.5
β-Naphth	22.3[1]
2-Py	20.5
3-Py	21.6
4-Py	18.6
$CH=CH_2$	22.5
CH=CHPh	20.2[51]
C≡CH	22.1
C≡CPh	17.8
COMe	12.5[5]
COPh	11.4[5]
C≡N	12.0[5]
OPh	27.9[5]
OMe	30.7[5]
$^+NMe_3$	19.4[5]
NO_2	7.1[5]
SMe	23.4[5]
SPh	20.5[5]
SO_2Ph	12.2[6]
PPh_2	20.2[3]
$SiMe_3$	26.1[26]
$SiPh_3$	21.3[26]
F	28.5[52]
Cl	23.8[52]
$Ph-SO_2-i-Pr$	32.1



31.8

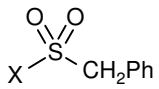


31.1[52]

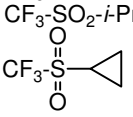


32.8[9]

Sulfones

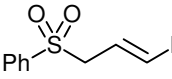


X = Me	25.4[55]
^{t}Bu	24.9[21]
NMePh	24.1[53]
CH_2Ph	23.9[52]
CF_3	14.6[52]
$CF_3-SO_2-CH_3$	18.8[2]
CF_3-SO_2-Et	20.4
CF_3-SO_2-i-Pr	21.8[2]



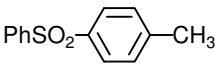
26.6[2]

$(CF_3-SO_2)_2CH_2$	2.1[52]
$Ph-SO_2-CHPh_2$	22.3[9]
$(PhSO_2)_2CHMe$	14.3[10]
$PhSO_2CH(SiMe_3)_2$	20.4[26]
$PhSO_2-CH_2CH=CH_2$	22.5[52]

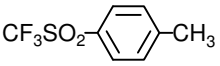


20.2[51]

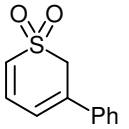
$PhSO_2-CH_2C≡CH$	22.1
$PhSO_2-CH_2C≡CPh$	17.8



29.8

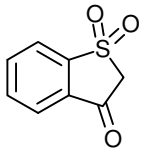


24.1



11.8[51]

$(MeSO_2)_2CH_2$	15.0[21]



10.1[53]

Author: Prof. Hans Reich

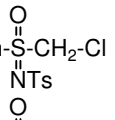
Updated 4/11/2022

Equilibrium pKa Table (DMSO Solvent and Reference)

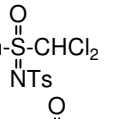
Halides

Ph-SO_2-CH_2-X

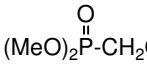
X = H	29.0[1]
F	28.5[52]
Cl	23.8



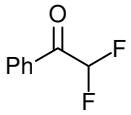
20.7



16.9

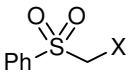


26.2

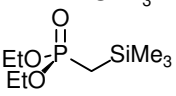


20.2[52]

Silanes (C-H)

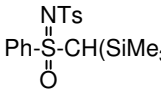


X = H	29.0[1]
$SiMe_3$	26.1[26]
$SiPh_3$	21.3[26]

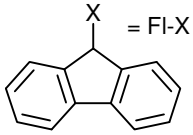


28.7[52]

$PhSO_2CH(SiMe_3)_2$ 20.4[26]



19.1[26]



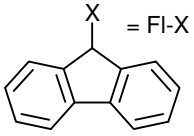
X = H	22.6[1]
Me	22.3[1]
$SiMe_3$	21.5[26]
$SiEt_3$	21.4[26]
$SiPh_3$	18.6[26]

Germanes (Ge-H)

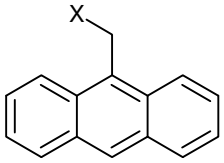
Ph_3Ge-H 23.1[63]

Ethers

PhO-CH_3	(49)[52]
MeO-CH_2COPh	22.9[5]
PhO-CH_2COPh	21.1[5]
MeO-CH_2SO_2Ph	30.7[5]
PhO-CH_2SO_2Ph	27.9[5]
PhO-CH_2C≡N	28.1[5]



X = H	22.6[21]
Ph	17.9[52]
MeO	22.1[5]
iPrO	21.4[5]
tBuO	21.3[5]
PhO	19.9[5]



X = H	31.1
OMe	30.6
OPh	30.2

Phosphines

Ph_2P-CH_2-PPh_2	29.9[3]
Ph_2P-CH_2-SO_2Ph	20.2[3]

Phosphonium (As) Salts

$Ph_3\overset{+}{P}$-CH_2-X

X = H	22.4[33]
Ph	17.4[33]
p-C_6H_4-CN	13.0[29]
p-C_6H_4-NO_2	11.0[29]
p-C_6H_4-OEt	18.8[29]
SPh	14.9[33]
CO_2Et	8.5[33]
COMe	7.1[33]
CHO	6.1[33]
CN	6.9[33]
COPh	6.0[33]

$Ph_3\overset{+}{P}$-CHMeCO_2Et 9.3[33]

$Ph_3\overset{+}{P}$-Pr-*i* 21.2

$Ph_3\overset{+}{P}$-CH_2-C_6H_4CN 13.0[29]

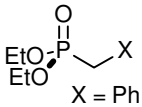
$Ph_3\overset{+}{As}$-CH_2-C_6H_4CN 17.0[29]

$Ph_3\overset{+}{P}$-CH_2-CH=CH_2 18.5[29]

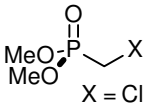
$Ph_3\overset{+}{P}CH_2$-CH=CHPh 15.6[29]

$Ph_3\overset{+}{P}$-Fl 6.6[33]

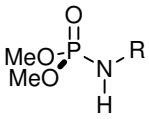
Phosphonates



X = Ph	27.6
C≡N	16.4
CO_2Et	18.6
Cl	26.2
$SiMe_3$	28.7[52]

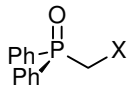


X = Cl 26.2

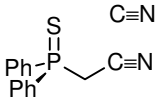


R = H	23.2
Me	24.9
Ph	18.3

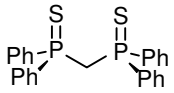
Phosphine Oxides



X = SPh	24.9
C≡N	16.9



16.3



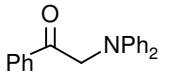
19.3

Author: Prof. Hans Reich

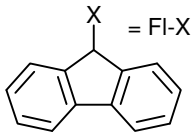
Updated 4/11/2022

Equilibrium pKa Table (DMSO Solvent and Reference)

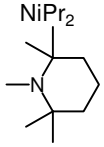
Amines (CH)



20.3[52]



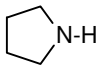
X =	H	22.6[52]
	NMe_2	22.5[36]
	NEt_2	21.4[36]
	$NiPr_2$	22.5[36]



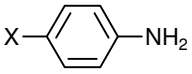
18.2[36]

Amines (NH)

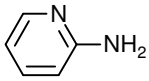
NH_3 (41)[19]



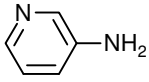
(44)[19]



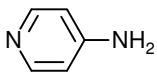
X =	H	30.6[11,54]
	m-CH_3	31.0[11,54]
	p-Ac	25.3[54]
	p-Bz	24.4[54]
	p-F	30.7[54]
	o-F	28.7[54]
	o-Cl	27.6[54]
	m-Cl	28.5[54]
	p-Cl	29.4[54]
	m-Br	28.4[54]
	p-Br	29.1[54]
	m-OMe	30.5[54]
	p-C≡N	25.3[11]
	m-C≡N	27.5[11]
	p-PhCO	24.4[11]
	p-PhS	28.2[54]
	p-$PhSO_2$	24.9[11,54]
	p-$MeSO_2$	25.6[54]
	p-CF_3SO_2	21.8[54]
	p-CF_3	27.0[54]
	m-CF_3	28.2[54]
	p-NO_2	20.9[11,54]



27.7[54]



28.5



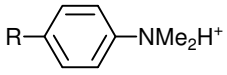
26.5[54]

$N≡C-NH_2$ 17.0[19]

Ph_2NH 25.0[16]

Ammonium Salts (NH)

NH_4^+	10.5[52]
$BuNH_3^+$	11.1[64]
$PhNH_3^+$	3.8[64]



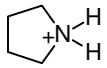
R =	H	2.4
	OMe	3.6
	Me	3.0

$Et_3\overset{+}{N}-H$ 9.0[47,64]

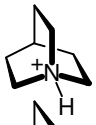
$Bn\overset{+}{N}H_3$ 10.2[64]

$BnMe_2\overset{+}{N}-H$ 7.6[47]

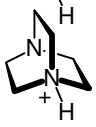
$Bn_3\overset{+}{N}-H$ 3.7[46]



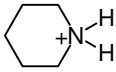
11.1[64]



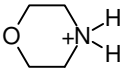
9.8[45]



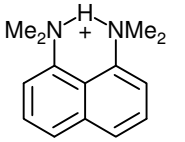
8.9[45,64]



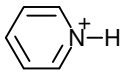
10.9[64]



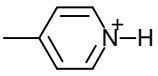
9.2[64]



7.5[45]

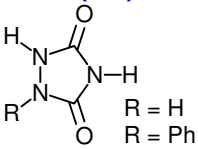


3.4[52]

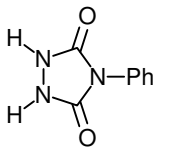


4.1

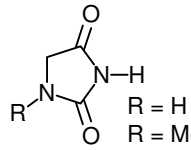
Imides (NH)



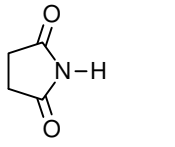
R = H	13.1[48]
R = Ph	9.9[48]



11.0[48]



R = H	15.1[48]
R = Me	15.0[48]



14.7

Ammonium Salts (CH)

$Me_3\overset{+}{N}-CH_2-X$

X =	H	(42)[33,44]
	SO_2Ph	19.4[5]
	C≡N	20.6[5]
	COMe	16.3[33]
	COPh	14.6[5]
	CO_2Et	20.0[33]
	$CONEt_2$	24.9[18]
	$CONEt_2$	15.3[27]
	Ph	31.9[33]
	SPh	28.0[33]

1-$Py\overset{+}{}-CH_2-X$

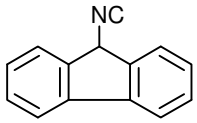
X =	C≡N	16.5[44]
	COMe	11.8[44]
	COPh	10.7[44]
	CO_2Et	14.1[44]
	$CONEt_2$	24.9[18]
	Ph	20.5[44]
	SPh	17.7[44]

$Me_3\overset{+}{N}-Fl$ 17.8[33]

Py+-Fl 11.8[44]

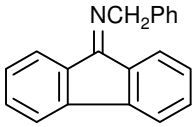
Isocyanide

$PhCH_2N=C$ 27.4[52]

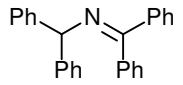


12.3[52]

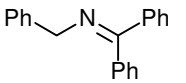
Imines (CH)



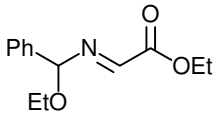
14.4



26.5

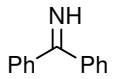


24.3[52]



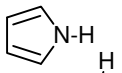
22.1

Imines (NH)

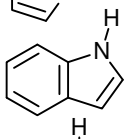


31.0[41]

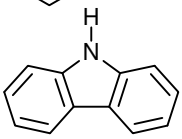
Pyrrole, Indole (N-H)



23.0[19]

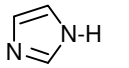


21.0[19]

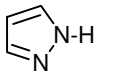


19.9[19]

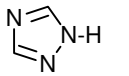
Azoles (NH)



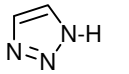
18.6[52]



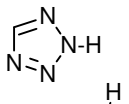
19.8[52]



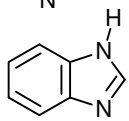
14.8[52]



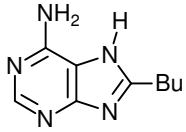
13.9[52]



8.2[52]

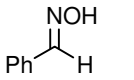


16.4[52]



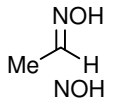
15.3

Oximes (OH)

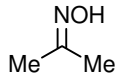


20.2[31]

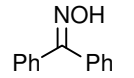
p-NO_2-C_6H_4 17.0[31]



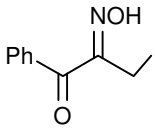
28.5[31]



25.2[31]



20.1[31]



14.9[31]

Author: Prof. Hans Reich

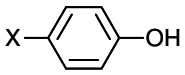
Updated 4/11/2022

Equilibrium pKa Table (DMSO Solvent and Reference)

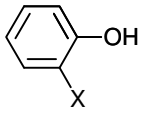
Alcohols (OH)

HOH	31.4[24]
MeOH	29.0[24]
EtOH	29.8[24]
i-PrOH	30.3[24]
t-BuOH	32.2[24]
CF_3CH_2OH	23.5[52]
$(CF_3)_2CHOH$	17.9
$(CF_3)_3COH$	10.7[52]

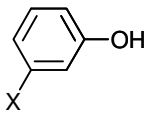
Phenols (OH)



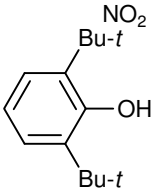
X =	
H	18.0[25]
Me	18.9[25]
OMe	19.1
OAc	14.1
NMe_2	19.8
NO_2	10.8
CF_3	15.3
Cl	16.7[25]
F	18.0
NMe_3^+	14.7
SO_2Me	13.6
CN	13.2



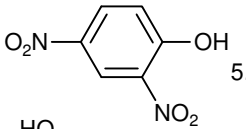
X =	
F	15.6
OMe	17.8
Ac	14.8
CN	12.1
NH_2	18.2



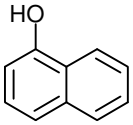
X =	
Cl	15.8[25]
F	15.8[25]
CN	14.8[25]
NO_2	14.4[25]



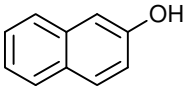
16.8



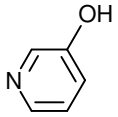
5.1



16.2

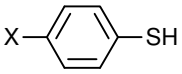


17.2



15.7

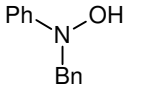
Thiols (SH)



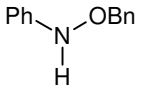
X =	
H	10.3[20]
OMe	11.2[20]
Br	9.0[20]
NO_2	5.5[20]

t-BuSH	17.9
n-BuSH	17.0
MeO_2CCH_2-SH	12.9
$PhCH_2$-SH	15.3
PhC(O)-SH	5.2[62]
Ph-SeH	7.1[62]

Hydroxylamine (NH, OH)



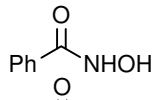
23.9



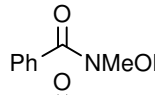
23.5

PhNHOH 24.2

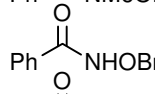
Hydroxamic Acid (NH,OH)



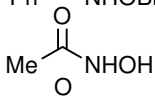
13.7[27]



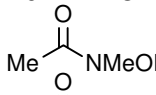
18.0[27]



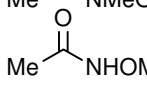
14.4[27]



16.0[27]



19.6[27]

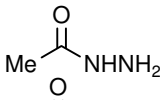


17.1[27]

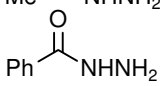
Inorganic Acids

HCN	12.9[52]
HN_3	7.9[52]
HF	15.[52]
HCl	1.8[52]
HBr	0.9[52]
NH_4^+	10.5[52]
HOH	31.4[24]
HON=O	7.5[52]
NH_3	(41)[19]
H_2N-CN	16.9[52]

Hydrazide (NH)

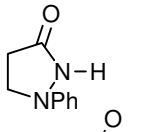


21.8[52]

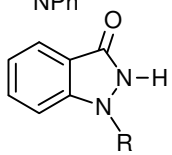


18.9[52]

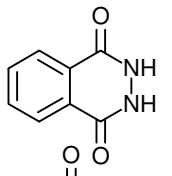
$PhSO_2$-$NHNH_2$	17.1[52]
$PhSO_2$-$NHNMe_2$	15.8[52]
Me(C=O)-$NHNH_2$	21.8[27]
Ac-NHNH-Ac	16.7[56]
Ph(C=O)-$NHNMe_2$	19.7
Ph(C=O)-$NHNH_2$	18.9[27]
Ph(C=O)-$NHNMe_2$	19.7[27]
3-Py(C=O)-$NHNH_2$	17.5[27]
EtO_2C-$NHNH_2$	22.2[56]
$O=C(NHNH_2)_2$	23.3[57]
$S=C(NHNH_2)_2$	16.6[57]



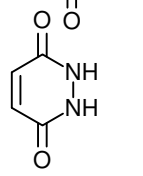
15.3[56]



R=H	14.9[56]
R=Ph	15.2[56]

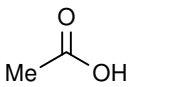


12.7[56]

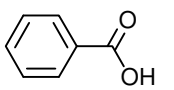


13.2[56]

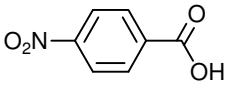
Carboxylic Acids (OH)



12.6[39]

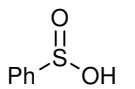


11.1[42]



9.1

Sulfinic Acids (OH)

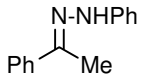


7.1

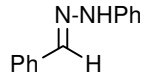
Sulfonic Acids (OH)

Me-SO_2-OH 1.6[39]

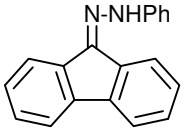
Hydrazone (NH)



21.6



21.1



14.9

Hydrazine (NH)

Ph-NHNH-Ph	26.2[56]
Ph-$NHNH_2$	28.8[56]
Ph-$NHNPh_2$	24.5[56]
2,4-$(NO_2)_2$PhNHNPh$_2$	12.1[56]
4-CF_3PhNHNH_2	25.7[56]
4-NC-PhNHNH_2	25.1[56]

Sulfonamide (NH)

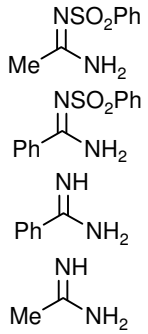
Me-SO_2-NH_2	17.5[39]
CF_3-SO_2-NH_2	9.7[39]
Ph-SO_2-NH_2	16.1[27]
Ph-SO_2-NHOH	15.4[57]
Me-SO_2-NHPh	12.9
Ph SO_2-$NHNH_2$	17.1[27]
Ph-SO_2-$NHNMe_2$	15.8[57]

24.3

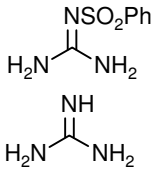
Author: Prof. Hans Reich

Updated 4/11/2022

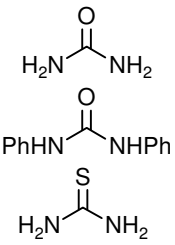
Amidine (NH)



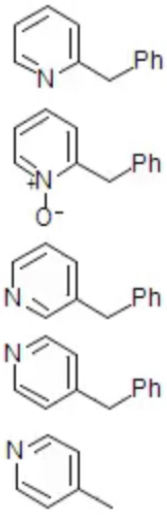
Guanidine (NH)

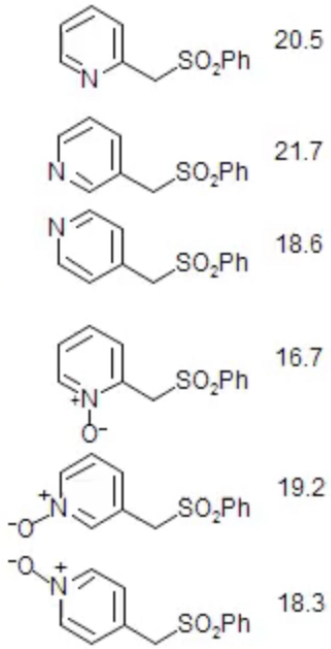


Ureas (NH)



Pyridyl





Equilibrium pKa Table (DMSO Solvent and Reference)

References (Bordwell et al.)

1. *J. Am. Chem. Soc.* **1975**, *97*, 7006.
2. *J. Am. Chem. Soc.* **1975**, *97*, 7160.
3. *J. Am. Chem. Soc.* **1975**, *97*, 442.
4. *J. Am. Chem. Soc.* **1967**, *89*, 2752.
5. *J. Org. Chem.* **1976**, *41*, 1885.
6. *J. Org. Chem.* **1976**, *41*, 1883.
7. *J. Org. Chem.* **1976**, *41*, 2786.
8. *J. Org. Chem.* **1976**, *41*, 2508.
9. *J. Org. Chem.* **1977**, *42*, 321.
10. *J. Org. Chem.* **1977**, *42*, 326.
11. *J. Org. Chem.* **1977**, *42*, 1817.
12. *J. Org. Chem.* **1978**, *43*, 3113.
13. *J. Org. Chem.* **1978**, *43*, 3095.
14. *J. Org. Chem.* **1978**, *43*, 1764.
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All others are F. G. Bordwell, private communication. For a review, see: F. G. Bordwell *Acc. Chem. Res.* **1988**, *21*, 456, 463.

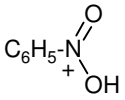
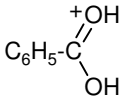
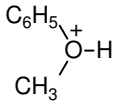
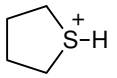
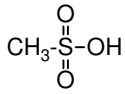
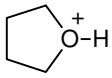
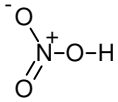
Author: Prof. Hans Reich

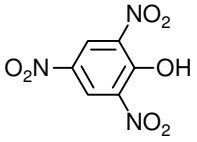
Updated 4/11/2022

Equilibrium pKa Table (H_2O Solvent and Reference)

Values outside the boxes were determined by approximate methods.

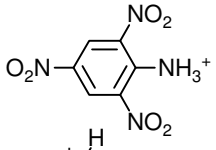
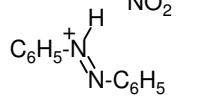
Oxygen Acids

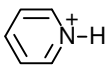
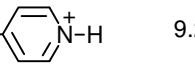
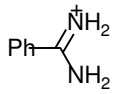
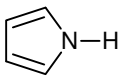
CF_3SO_3H	
	-12.4
	-7.8
	-6.5
$(CH_3)_2\overset{+}{S}-H$	-5.4
	-4.4
$(CH_3)_2\overset{+}{O}-H$	-3.8
	-2.6
$CH_3-\overset{+}{O}H_2$	-2.2
	-2.1
$(CH_3)_2S=\overset{+}{O}H$	-1.8
	-1.4
CF_3-CO_2H	-0.3

	0.3
$(CH_3)_2Se=\overset{+}{O}H$	2.6
$C_6H_5-CO_2H$	4.2
CH_3CO_2H	4.8
$HOCO_2H$	6.3
C_6H_5-SH	6.5
$CH_2=C(Ph)OH$	8.0[2]
C_6H_5-OH	10.0
HCO_3^-	10.3
RS-H	10.5
$CH_2=CHOH$	10.5
$CH_2=C(CH_3)OH$	10.9
HOOH	11.7
H_2O	14.0[10]
CH_3-OH	16

$(CH_3)_3C-OH$ 20

Nitrogen Acids

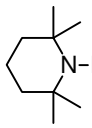
$\overset{+}{P}H_4$	-14.
$C_6H_5-C\equiv\overset{+}{N}-H$	-10.5
$CH_3-C\equiv\overset{+}{N}-H$	-10.
	-9.3
	-2.9

$(C_6H_5)_2\overset{+}{N}H_2$	0.8
$CH_3-\overset{+}{P}H_3$	2.7
$C_6H_5-\overset{+}{N}H_3$	4.6
	5.2
$N\equiv C-CH_2CH_2-\overset{+}{N}H_3$	7.9
$(CH_3CH_2)_3\overset{+}{P}-H$	9.1
	9.2
$\overset{+}{N}H_4$	9.2
$N\equiv\overset{+}{N}-H$	10.0
$CH_3CH_2\overset{+}{N}H_3$	10.6
$(CH_3CH_2)_2\overset{+}{N}H_2$	11.0
$(CH_3CH_2)_3\overset{+}{N}H$	10.8
O=N-H	11.5
	11.2[4]
$(CH_3)_2N-\overset{+}{C}(=NH_2)-N(CH_3)_2$	13.6
	15.

$C_6H_5-NH_2$ 28.

$((CH_3)_3Si)_2N-H$ 30.

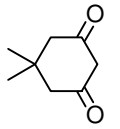
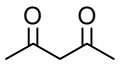
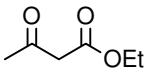
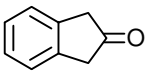
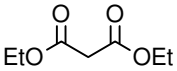
$(i\text{-}C_3H_7)_2N-H$ 36.

 37.

Halogen Acids

H-I	-5.2
H-Br	-4.7
H-Cl	-2.2
H-F	3.2

Carbon Acids

$(O_2N)_2CH_2$	3.6
	5.2
	9.0[3]
N≡C-H	9.1
$CH_3\overset{+}{N}\equiv N$	10.0[1]
O_2N-CH_3	10.2
	10.7
$(CF_3)_3CH$	11.
$(NC)_2CH_2$	11.2
	12.2[6]
	12.9
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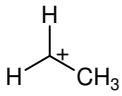
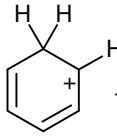
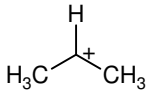
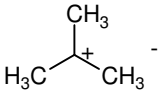
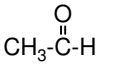
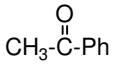
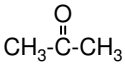
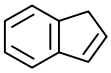
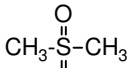
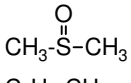
 -24.8

 -24.3

 -18.5

 -12.5

	16.7
	18.3
	19.3
	20
$C_6H_5-CH_2-C\equiv N$	21
$C_6H_5-C\equiv C-H$	23
CH_3CO_2Et	24
H-C≡C-H	24
$CH_3-C\equiv N$	25
	29
CF_3-H	32
	33
$(C_6H_5)_3C-H$	32
	33
$C_6H_5-CH_3$	41
	44
CH_3CH_3	50

Author: Prof. Hans Reich

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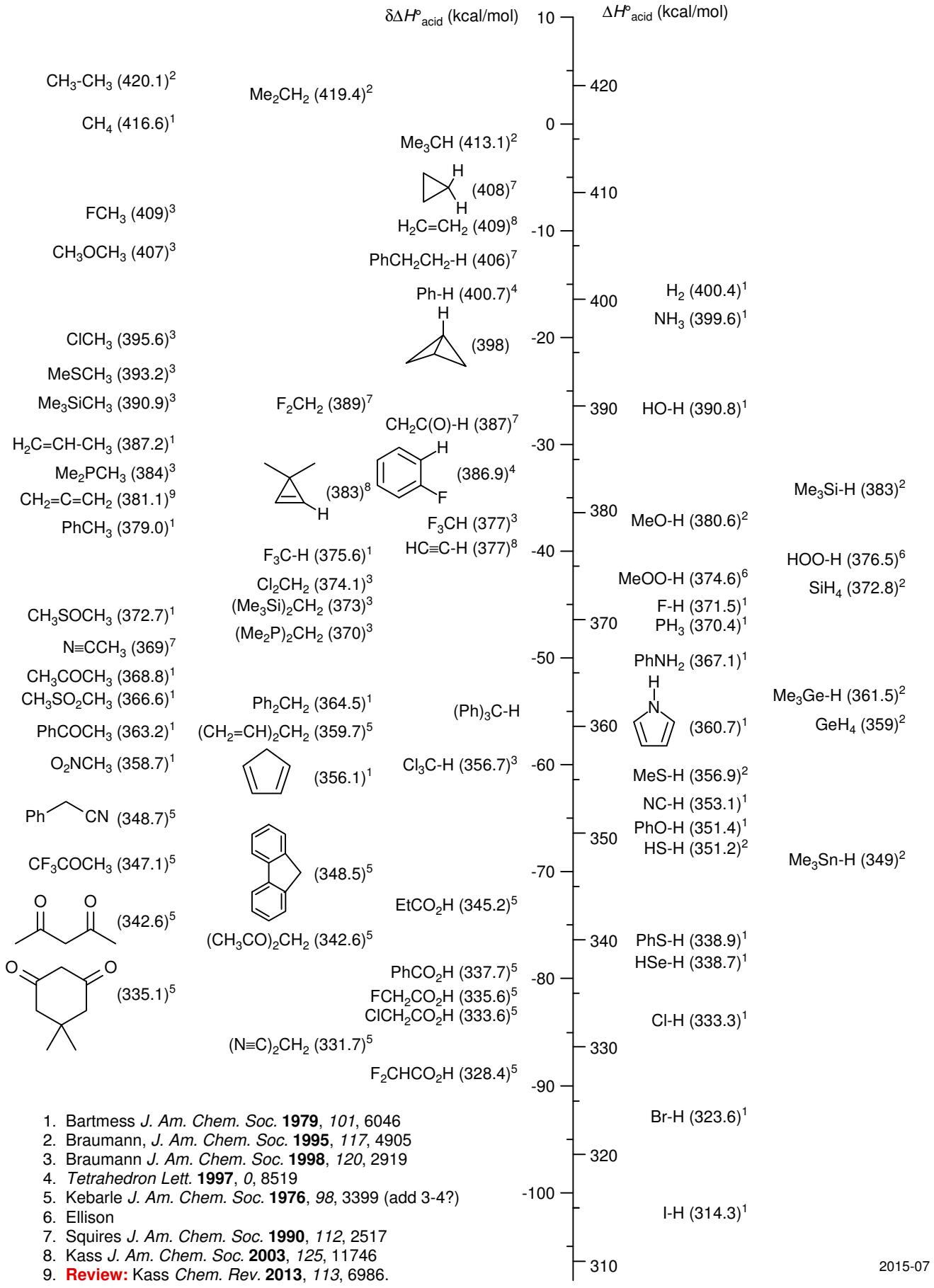
Gas Phase Acidities



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6. Ellison
7. Squires *J. Am. Chem. Soc.* **1990**, *112*, 2517
8. Kass *J. Am. Chem. Soc.* **2003**, *125*, 11746
9. **Review:** Kass *Chem. Rev.* **2013**, *113*, 6986.
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