PROTON AFFINITIES

Proton affinity is a useful parameter for describing gas phase ion-molecule reactions in fields such as atmospheric chemistry, plasma chemistry, mass spectrometry, and astrophysics. The proton affinity E_{pa} (often designated in the literature as PA) of a molecular species M is defined as the negative of the enthalpy change for the gas phase reaction

$$M + H^+ \rightarrow MH^+.$$

A closely related quantity is the gas phase basicity $\Delta_{base}G°$ (often designated as GB), which is the negative of the Gibbs energy change for the same reaction. Thus the two are related by

$$\Delta_{base}G° = E_{pa} + T\Delta S,$$

where T is the temperature and ΔS is the entropy change in the reaction (which can be calculated if the molecular structure of M and M^+ is known).

Direct measurement of the proton affinity is possible for only a few molecules, mainly olefins and carbonyl compounds. However, these measurements have been used to establish a scale of E_{pa} values that permits proton affinities to be determined for many other molecules, including unstable species and reaction intermediates. The basis for this scale is described by Hunter and Lias in Reference 1.

The E_{pa} and $\Delta_{base}G°$ values at a temperature of 298 K are tabulated below for selected molecules. Many values are given to one decimal place, but the majority are not accurate to better than one or two kilojoules per mole. The methods of measurement are described in Reference 1, which contains a much more extensive and detailed tabulation.

Compounds are listed by molecular formula in the Hill order, but with all compounds that do not contain carbon appearing before those that do contain carbon.

References

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Molecular formula	Name	E_{pa} kJ/mol	$\Delta_{base}G°$ kJ/mol	Notes
Ar	Argon	369.2	346.3	
AsF_3	Arsenic(III) fluoride	636.7	604.2	
AsH_3	Arsine	747.9	712.0	
BHO_2	Metaboric acid	763.0	730.5	
BH_3O_3	Boric acid	728.1	698.4	
B_2H_6	Diborane	615	586.0	
$B_3H_6N_3$	Borazine	802.5	772.8	
B_4H_{10}	Tetraborane(10)	605	572.5	
B_5H_9	Pentaborane(9)	699.4	666.9	
BaO	Barium oxide	1215.4	1187.6	
Br	Bromine (atomic)	554.4	531.2	
BrH	Hydrogen bromide	584.2	557.7	
BrLi	Lithium bromide	819	792.5	
CaO	Calcium oxide	1190.6	1162.3	
Cl	Chlorine (atomic)	513.6	490.1	
ClH	Hydrogen chloride	556.9	530.1	
ClLi	Lithium chloride	827	800.5	
Co	Cobalt	742.7	719.8	
Cr	Chromium	791.3	768.4	
CsHO	Cesium hydroxide	1117.9	1092.2	
Cs_2O	Cesium oxide	1442.9	1412.2	
Cu	Copper	655.3	632.4	
F	Fluorine (atomic)	340.1	315.1	
FH	Hydrogen fluoride	484	456.7	
FO	Fluorine oxide	508.7	482.2	
F_2	Fluorine	332	305.5	
F_2O_2S	Sulfuryl fluoride	605.5	580.5	

Molecular formula	Name	E_{pa} kJ/mol	$\Delta_{base}G°$ kJ/mol	Notes
F_3N	Nitrogen trifluoride	568.4	538.6	
F_3OP	Phosphoryl fluoride	694.0	664.2	
F_3P	Phosphorus(III) fluoride	695.3	662.8	
F_4Si	Tetrafluorosilane	502.9	476.6	
F_6S	Sulfur hexafluoride	575.3	550.7	
Fe	Iron	754	731.1	
FeO	Iron(II) oxide	907	880.5	
GeH_4	Germane	713.4	687.1	
HI	Hydrogen iodide	627.5	601.3	
HKO	Potassium hydroxide	1101.8	1075.4	
HLi	Lithium hydride	1021.7	996.4	
HLiO	Lithium hydroxide	1000.1	972.1	
HNO_3	Nitric acid	751.4	731.5	
HN_3	Hydrazoic acid	756.0	723.5	
HNa	Sodium hydride	1095	1070.6	
HNaO	Sodium hydroxide	1071.8	1044.8	
HO	Hydroxyl	593.2	564.0	
HO_2	Hydroperoxy	660	627.5	
HP	Phosphorus monohydride	670.3	639.6	
H_2	Hydrogen	422.3	394.7	
$H_2N_2O_2$	Nitramide	757.4	725.0	
H_2O	Water	691	660.0	
H_2O_2	Hydrogen peroxide	674.5	643.8	
H_2O_4S	Sulfuric acid	717	681	Ref. 3
H_2P	Phosphino	709.2	675.7	
H_2S	Hydrogen sulfide	705	673.8	
H_2Se	Hydrogen selenide	707.8	676.4	
H_2Si	Silylene	839.2	804.1	
H_2Te	Hydrogen telluride	735.9	704.5	
H_3N	Ammonia	853.6	819.0	
H_3P	Phosphine	785	750.9	
H_4N_2	Hydrazine	853.2	822.4	
H_4Si	Silane	639.7	613.4	
H_6OSi_2	Disiloxane	749	718.3	
He	Helium	177.8	148.5	
I	Iodine (atomic)	608.2	583.5	
K_2O	Potassium oxide	1342.5	1311.8	
Kr	Krypton	424.6	402.4	
La	Lanthanum	1013	991.9	
Li_2	Dilithium	1162	1133.1	
Li_2O	Lithium oxide	1206	1175.3	
Lu	Lutetium	992	970.6	
Mg	Magnesium	819.6	797.3	
MgO	Magnesium oxide	988	959.4	
Mg_2	Dimagnesium	919	886.5	
Mn	Manganese	797.3	774.4	
N	Nitrogen (atomic)	342.2	318.7	
NO	Nitric oxide	531.8	505.3	
NO_2	Nitrogen dioxide	591.0	560.3	
NP	Phosphorus nitride	789.4	757.0	
N_2	Nitrogen	493.8	464.5	
N_2O	Nitrous oxide	549.8	523.3	Protonation at N
N_2O	Nitrous oxide	575.2	548.7	Protonation at O
Na_2	Disodium	1146.8	1118.2	
Na_2O	Sodium oxide	1375.9	1345.2	
Ne	Neon	198.8	174.4	
Ni	Nickel	737	714.1	
O	Oxygen (atomic)	485.2	459.6	
OP	Phosphorus monoxide	682	649.5	
OSi	Silicon monoxide	777.8	750.4	Protonation at O

Molecular formula	Name	E_{pa} kJ/mol	$\Delta_{base}G°$ kJ/mol	Notes
OSi	Silicon monoxide	533	500.5	Protonation at Si
OSr	Strontium oxide	1209	1180.7	
O_2	Oxygen	421	396.3	
O_2S	Sulfur dioxide	672.3	643.3	
O_3	Ozone	625.5	595.9	
O_3S	Sulfur trioxide	588.3	560.3	
O_4Os	Osmium(VIII) oxide	676.9	650.6	
P	Phosphorus	626.8	604.8	
Pd	Palladium	696	673.4	
Rh	Rhodium	768	745.4	
Ru	Ruthenium	774	751.4	
S	Sulfur	664.3	640.2	
SSi	Silicon monosulfide	627	596.6	Protonation at Si
SSi	Silicon monosulfide	683	660.2	Protonation at S
Sc	Scandium	914	892.0	
Si	Silicon	837	814.1	
Ti	Titanium	876	853.7	
U	Uranium	995.2	973.2	
V	Vanadium	859.4	836.8	
Xe	Xenon	499.6	478.1	
Y	Yttrium	967	945.9	
Zn	Zinc	608.6	586.0	
$CBrF_3$	Bromotrifluoromethane	580.0	550.3	
CBrN	Cyanogen bromide	749.8	719.2	
$CClF_3$	Chlorotrifluoromethane	571.3	541.5	
CClN	Cyanogen chloride	722.1	691.5	
CCl_2	Dichloromethylene	861	828.5	
CCl_2S	Carbonothioic dichloride	752.5	721.8	
CFN	Cyanogen fluoride	632	601.3	
CF_2	Difluoromethylene	765	732.5	
CF_2O	Carbonyl fluoride	666.7	637.0	
CF_3I	Trifluoroiodomethane	628.0	598.2	
CF_3NO	Trifluoronitrosomethane	703.3	670.8	
CF_4	Tetrafluoromethane	529.3	503.7	
CHCl	Chloromethylene	874.1	839.9	
CHF	Fluoromethylene	797.9	763.8	
CHF_3	Trifluoromethane	619.5	589.7	
CHF_3O_3S	Trifluoromethanesulfonic acid	699.4	666.9	
CHN	Hydrogen cyanide	712.9	681.6	
CHN	Hydrogen isocyanide	772.3	739.8	
CHNO	Isocyanic acid (HNCO)	753	718.8	
CHNO	Fulminic acid	758	725.5	
CHO	Oxomethyl (HCO)	636	601.8	
CHO_2	Formyloxyl	623.4	590.9	
CH_2F_2	Difluoromethane	620.5	589.7	
CH_2N_2	Diazomethane	858.9	826.7	
CH_2N_2	Cyanamide	805.6	774.9	
CH_2O	Formaldehyde	712.9	683.3	
CH_2O_2	Formic acid	742.0	710.3	
CH_2S	Thioformaldehyde	759.7	730.5	
CH_2Se	Selenoformaldehyde	764.0	734.9	
CH_3Br	Bromomethane	664.2	638.0	
CH_3Cl	Chloromethane	647.3	621.1	
CH_3F	Fluoromethane	598.9	571.5	
CH_3I	Iodomethane	691.7	665.5	
CH_3NO	Formamide	822.2	791.2	
CH_3NO_2	Nitromethane	754.6	721.6	
CH_3NO_2	Methyl nitrite	798.9	766.4	
CH_3NO_3	Methyl nitrate	733.6	714.8	
CH_3N_3	Methyl azide	833	800.5	

Molecular formula	Name	E_{pa} kJ/mol	$\Delta_{base}G°$ kJ/mol	Notes
CH_4	Methane	543.5	520.6	
CH_4N	Methylamidogen	832.8	801.6	
CH_4N_2O	Urea	873.5	841.6	Protonation at O; Ref. 8
CH_4N_2S	Thiourea	893.7	863.9	
CH_4O	Methanol	754.3	724.5	
CH_4O_3S	Methanesulfonic acid	761.3	728.9	
CH_4S	Methanethiol	773.4	742	
CH_5N	Methylamine	899.0	864.5	
CH_5NO	*O*-Methylhydroxylamine	844.8	812.3	
CH_5N_3	Guanidine	986.3	949.4	
CH_5P	Methylphosphine	851.5	817.6	
CH_6N_2	Methylhydrazine	898.8	866.4	
CN	Cyanide	>595	>564	Protonation at N
CNS	Thiocyanate	751	718.5	
CO	Carbon monoxide	594	562.8	Protonation at C
CO	Carbon monoxide	426.3	402.2	Protonation at O
COS	Carbon oxysulfide	628.5	602.6	Protonation at S
COSe	Carbon oxyselenide	670	644.1	Protonation at Se
CO_2	Carbon dioxide	540.5	515.8	
CS	Carbon monosulfide	791.5	760	
CS_2	Carbon disulfide	681.9	657.7	
CSe	Carbon monoselenide	831.8	800.2	Protonation at C
CSe_2	Carbon diselenide	725	700.9	
C_2ClF_3O	Trifluoroacetyl chloride	681.6	649.8	
C_2Cl_3N	Trichloroacetonitrile	723.2	692.6	
C_2F_3N	Trifluoroacetonitrile	688.4	657.7	
C_2H	Ethynyl	753	720.8	
C_2HCl_3O	Trichloroacetaldehyde	722.3	690.5	
$C_2HCl_3O_2$	Trichloroacetic acid	770.0	739.1	
C_2HF	Fluoroacetylene	686	661.3	
C_2HF_3	Trifluoroethene	699.4	666.9	
$C_2HF_3O_2$	Trifluoroacetic acid	711.7	680.7	
C_2H_2	Acetylene	641.4	616.7	
C_2H_2ClN	Chloroacetonitrile	745.7	715.1	
$C_2H_2F_2$	1,1-Difluoroethene	734	705.1	
$C_2H_2F_2$	*trans*-1,2-Difluoroethene	688.6	657.9	
C_2H_2O	Ketene	825.3	793.6	
$C_2H_3ClO_2$	Chloroacetic acid	765.4	734.5	
$C_2H_3Cl_3O$	2,2,2-Trichloroethanol	729.3	698.9	
C_2H_3F	Fluoroethene	729	700.1	
$C_2H_3FO_2$	Fluoroacetic acid	765.4	734.5	
$C_2H_3F_3O$	2,2,2-Trifluoroethanol	700.2	669.9	
$C_2H_3F_3O$	Methyl trifluoromethyl ether	719.2	690.0	
C_2H_3N	Acetonitrile	779.2	748	
C_2H_3N	Isocyanomethane	839.1	806.6	
C_2H_3NO	Methyl isocyanate	764.4	732.0	
C_2H_3NS	Methyl thiocyanate	796.7	766.1	
C_2H_3NS	Methyl isothiocyanate	799.2	766.7	
$C_2H_3N_3$	1*H*-1,2,3-Triazole	879.3	847.4	
$C_2H_3N_3$	1*H*-1,2,4-Triazole	886.0	855.9	
C_2H_4	Ethylene	680.5	651.5	
$C_2H_4F_2O$	2,2-Difluoroethanol	727.4	697.0	
$C_2H_4F_3N$	2,2,2-Trifluoroethylamine	846.8	812.9	
$C_2H_4N_2$	Aminoacetonitrile	824.9	791.0	
C_2H_4O	Acetaldehyde	768.5	736.5	
C_2H_4O	Oxirane	774.2	745.3	
$C_2H_4O_2$	Acetic acid	783.7	752.8	
$C_2H_4O_2$	Methyl formate	782.5	751.5	
C_2H_4S	Thiirane	807.4	777.6	
C_2H_5Br	Bromoethane	696.2	669.7	

Molecular formula	Name	E_{pa} kJ/mol	$\Delta_{base}G°$ kJ/mol	Notes
C_2H_5BrO	2-Bromoethanol	766.1	735.7	
C_2H_5Cl	Chloroethane	693.4	666.9	
C_2H_5ClO	2-Chloroethanol	766.1	735.7	
C_2H_5F	Fluoroethane	683.4	655.8	
C_2H_5FO	2-Fluoroethanol	715.6	685.2	
C_2H_5I	Iodoethane	724.8	698.3	
C_2H_5N	Ethenamine	898.9	866.5	
C_2H_5N	Ethyleneimine	905.5	872.5	
C_2H_5NO	Acetamide	863.6	832.6	
C_2H_5NO	*N*-Methylformamide	851.3	820.3	
$C_2H_5NO_2$	Nitroethane	765.7	733.2	
$C_2H_5NO_2$	Ethyl nitrite	818.9	786.4	
$C_2H_5NO_2$	Glycine	886.5	852.2	
$C_2H_5NO_2$	Acetohydroxamic acid	854.0	823.0	
C_2H_5NS	Thioacetamide	884.6	852.8	
C_2H_6	Ethane	596.3	569.9	
C_2H_6Hg	Dimethyl mercury	771.6	740.8	
$C_2H_6N_2$	Ethanimidamide	970.7	938.2	
$C_2H_6N_2$	trans-Dimethyldiazene	865.1	834.4	
$C_2H_6N_2O$	2-Aminoacetamide		882.3	
$C_2H_6N_2O_2$	*N*-Methyl-*N*-nitromethanamine	828.3	795.8	
C_2H_6O	Ethanol	776.4	746	
C_2H_6O	Dimethyl ether	792	764.5	
C_2H_6OS	Dimethyl sulfoxide	884.4	853.7	
$C_2H_6O_2$	1,2-Ethanediol	815.9	773.6	
C_2H_6S	Ethanethiol	789.6	758.4	
C_2H_6S	Dimethyl sulfide	830.9	801.2	
$C_2H_6S_2$	Dimethyl disulfide	815.3	782.8	
C_2H_7N	Ethylamine	912.0	878	
C_2H_7N	Dimethylamine	929.5	896.5	
C_2H_7NO	Ethanolamine	930.3	896.8	
$C_2H_7O_3P$	Dimethyl hydrogen phosphite	894.8	862.4	
C_2H_7P	Dimethylphosphine	912.0	877.9	
$C_2H_8N_2$	1,2-Ethanediamine	951.6	912.5	
$C_2H_8N_2$	1,1-Dimethylhydrazine	927.1	894.7	
C_2N_2	Cyanogen	674.7	645.8	
C_2O	Dicarbon monoxide	774.7	747.0	
C_3	Carbon trimer	767.0	736.3	
C_3F_6O	Perfluoroacetone	670.4	639.7	
C_3HN	Cyanoacetylene	751.2	720.5	
$C_3H_2F_6O$	1,1,1,3,3,3-Hexafluoro-2-propanol	686.6	656.2	
$C_3H_2N_2$	Malononitrile	723.0	694.1	
C_3H_3	2-Propynyl	741	708.5	
$C_3H_3Cl_3O$	1,1,1-Trichloro-2-propanone	768.3	736.3	
$C_3H_3F_3O$	1,1,1-Trifluoroacetone	723.9	692.0	
$C_3H_3F_3O_2$	Methyl trifluoroacetate	740.5	709.6	
C_3H_3N	Acrylonitrile	784.7	753.7	
C_3H_3NO	Oxazole	876.4	844.5	
C_3H_3NO	Isoxazole	848.6	816.8	
C_3H_3NO	2-Oxopropanenitrile	746.9	716.2	
C_3H_3NS	Thiazole	904	872.1	
$C_3H_3N_3$	1,3,5-Triazine	848.8	819.6	
C_3H_4	Allene	775.3	745.8	
C_3H_4	Propyne	748.2	723.0	
C_3H_4	Cyclopropene	818.5	787.8	
C_3H_4ClN	3-Chloropropanenitrile	773.1	742.4	
$C_3H_4N_2$	1*H*-Pyrazole	894.1	860.5	
$C_3H_4N_2$	Imidazole	942.8	909.2	
$C_3H_4N_2S$	2-Thiazolamine	930.6	898.7	
C_3H_4O	Acrolein	797.0	765.1	

Molecular formula	Name	E_{pa} kJ/mol	$\Delta_{base}G°$ kJ/mol	Notes
C_3H_4O	1-Propen-1-one	834.1	803.4	
$C_3H_4O_3$	Ethylene carbonate	814.2	784.4	
C_3H_5	Allyl	736	707.4	
C_3H_5	Cyclopropyl	738.9	702.0	
$C_3H_5ClO_2$	Ethyl chloroformate	764.8	733.8	
C_3H_5FO	1-Fluoro-2-propanone	795.4	763.5	
$C_3H_5F_3O$	2,2,2-Trifluoroethyl methyl ether	747.6	718.4	
C_3H_5N	Propanenitrile	794.1	763.0	
C_3H_5N	2-Propyn-1-amine	887.4	853.5	
C_3H_5N	Ethyl isocyanide	851.3	818.9	
C_3H_5NO	Acrylamide	870.7	839.8	
C_3H_5NO	Methoxyacetonitrile	758.1	727.4	
C_3H_5NO	2-Azetidinone	852.6	821.7	
C_3H_5NS	(Methylthio)acetonitrile	784.8	754.1	
$C_3H_5N_3$	1*H*-Pyrazol-3-amine	921.5	889.6	
$C_3H_5N_3$	1*H*-Pyrazol-4-amine	907.6	874.0	
C_3H_6	Propene	741.6		Ref. 5
C_3H_6	Cyclopropane	750.3	722.2	
$C_3H_6N_2$	3-Aminopropanenitrile	866.4	832.5	
$C_3H_6N_2$	Dimethylcyanamide	852.1	821.4	
$C_3H_6N_2S$	2-Imidazolidinethione	921.9	891.2	
C_3H_6O	Methyl vinyl ether	859.2	830.3	
C_3H_6O	Propanal	786.0	754.0	
C_3H_6O	Acetone	812	782.1	
C_3H_6O	Oxetane	801.3	773.9	
$C_3H_6O_2$	Propanoic acid	797.2	766.2	
$C_3H_6O_2$	Ethyl formate	799.4	768.4	
$C_3H_6O_2$	Methyl acetate	821.6	790.7	
$C_3H_6O_3$	Dimethyl carbonate	830.2	799.2	
C_3H_6S	(Methylthio)ethene	858.2	829.3	
C_3H_6S	Thietane	834.8	805.0	
C_3H_6S	Methylthiirane	833.3	801.5	
C_3H_7N	Allylamine	909.5	875.5	
C_3H_7N	Cyclopropylamine	904.7	869.9	
C_3H_7N	Azetidine	943.4	908.6	
C_3H_7N	1-Methylaziridine	934.8	904.1	
C_3H_7N	Propyleneimine	925.1	892.1	
C_3H_7NO	*N,N*-Dimethylformamide	887.5	856.6	
C_3H_7NO	*N*-Methylacetamide	888.5	857.6	
C_3H_7NO	Propanamide	876.2	845.3	
$C_3H_7NO_2$	Isopropyl nitrite	845.5	813.0	
$C_3H_7NO_2$	*L*-Alanine	901.6	867.7	
$C_3H_7NO_2$	Sarcosine	921.2	888.7	
$C_3H_7NO_2S$	*L*-Cysteine	903.2	869.3	
$C_3H_7NO_3$	*L*-Serine	914.6	880.7	
C_3H_8	Propane	625.7	607.8	
$C_3H_8N_2O$	*N,N'*-Dimethylurea	903.3	873.5	
$C_3H_8N_2S$	*N,N'*-Dimethylthiourea	926.0	895.1	
C_3H_8O	1-Propanol	786.5	756.1	
C_3H_8O	2-Propanol	793.0	762.6	
C_3H_8O	Ethyl methyl ether	808.6	781.2	
$C_3H_8O_2$	1,3-Propanediol	876.2	825.9	
$C_3H_8O_2$	2-Methoxyethanol	768.8	729.8	
$C_3H_8O_3$	Glycerol	874.8	820	
C_3H_8S	1-Propanethiol	794.9	763.6	
C_3H_8S	2-Propanethiol	803.6	772.3	
C_3H_8S	Ethyl methyl sulfide	846.5	815.3	
C_3H_9As	Trimethylarsine	897.3	864.9	
$C_3H_9BO_3$	Trimethyl borate	815.8	783.4	
C_3H_9N	Propylamine	917.8	883.9	

Molecular formula	Name	E_{pa} kJ/mol	$\Delta_{base}G°$ kJ/mol	Notes
C_3H_9N	Isopropylamine	923.8	889.0	
C_3H_9N	Ethylmethylamine	942.2	909.2	
C_3H_9N	Trimethylamine	948.9	918.1	
C_3H_9NO	2-Methoxyethylamine	928.6	894.6	
C_3H_9NO	Trimethylamine oxide	983.2	953.5	
C_3H_9NO	3-Amino-1-propanol	962.5	917.3	
$C_3H_9O_3P$	Trimethyl phosphite	929.7	899.9	
$C_3H_9O_4P$	Trimethyl phosphate	890.6	860.8	
C_3H_9P	Trimethylphosphine	958.8	926.3	
$C_3H_{10}N_2$	1,3-Propanediamine	987.0	940.0	
$C_3H_{10}OSi$	Trimethylsilanol	814.0	781.5	
C_4F_8	Perfluorocyclobutane	>544		Ref. 6
C_4H_2	1,3-Butadiyne	737.2	712.8	
$C_4H_4F_6O$	Bis(2,2,2-trifluoroethyl) ether	702.3	674.9	
$C_4H_4N_2$	Pyrazine	877.1	847.0	
$C_4H_4N_2$	Pyrimidine	885.8	855.7	
$C_4H_4N_2$	Pyridazine	907.2	877.1	
$C_4H_4N_2O_2$	Uracil	872.7	841.7	
$C_4H_4N_2S_2$	2,4(1*H*,3*H*)-Pyrimidinedithione	911.4	880.5	
C_4H_4O	Furan	812	781	Ref. 10
$C_4H_4O_3$	Succinic anhydride	797		Ref. 9
C_4H_4S	Thiophene	815.0	784.3	
$C_4H_5Cl_3O_2$	Ethyl trichloroacetate	790.4	759.4	
$C_4H_5F_3O_2$	Ethyl trifluoroacetate	758.8	727.9	
C_4H_5N	Pyrrole	875.4	843.8	
C_4H_5N	Cyclopropanecarbonitrile	808.2	777.5	
$C_4H_5NO_2$	Ethyl cyanoformate	745.7	714.7	
C_4H_5NS	2-Methylthiazole	930.6	898.7	
$C_4H_5N_3O$	Cytosine	949.9	918	
C_4H_6	1,2-Butadiene	778.9	749.8	
C_4H_6	1,3-Butadiene	783.4	757.6	
C_4H_6	2-Butyne	775.8	745.1	
C_4H_6	Cyclobutene	784.4	753.6	
$C_4H_6F_3NO$	2,2,2-Trifluoro-*N,N*-dimethylacetamide	849.0	818.0	
$C_4H_6N_2$	1-Methylimidazol	959.6	927.7	
$C_4H_6N_2$	2-Methyl-1*H*-imidazole	963.4	929.6	
$C_4H_6N_2$	4-Methyl-1*H*-imidazole	952.8	920.9	
$C_4H_6N_2$	1-Methyl-1*H*-pyrazole	912.0	880.1	
$C_4H_6N_2$	3-Methyl-1*H*-pyrazole	906.0	874.2	
$C_4H_6N_2$	4-Methyl-1*H*-pyrazole	906.8	873.4	
C_4H_6O	2-Methylpropenal	808.7	776.8	
C_4H_6O	3-Buten-2-one	834.7	802.8	
C_4H_6O	Cyclobutanone	802.5	772.7	
C_4H_6O	2,3-Dihydrofuran	866.9	834.4	
C_4H_6O	2,5-Dihydrofuran	823.4	796	
$C_4H_6O_2$	*trans*-2-Butenoic acid	824.0	793	
$C_4H_6O_2$	Methacrylic acid	816.7	785.7	
$C_4H_6O_2$	Cyclopropanecarboxylic acid	821.4	790.4	
$C_4H_6O_2$	Vinyl acetate	813.9	782.9	
$C_4H_6O_2$	Methyl acrylate	825.8	794.8	
$C_4H_6O_2$	2,3-Butanedione	801.9	770.1	
$C_4H_6O_2$	γ-Butyrolactone	840.0	808.1	
$C_4H_6O_2$	2,3-Dihydro-1,4-dioxin	823.5	792.8	
$C_4H_6O_3$	Acetic anhydride	844		Ref. 9
C_4H_7	2-Methylallyl	778	747.3	
C_4H_7N	Butanenitrile	798.4	767.7	
C_4H_7N	2-Methylpropanenitrile	803.6	772.8	
C_4H_7N	1-Isocyanopropane	856.8	824.3	
C_4H_7NO	2-Butenamide	887.1	856.1	

Molecular formula	Name	E_{pa} kJ/mol	$\Delta_{base}G°$ kJ/mol	Notes
C_4H_7NO	2-Methyl-2-propenamide	880.4	849.4	
$C_4H_7NO_4$	*L*-Aspartic acid	908.9	875	
C_4H_8	*trans*-2-Butene	747	719.9	
C_4H_8	Isobutene	802.1	775.6	
$C_4H_8N_2$	(Dimethylamino)acetonitrile	884.5	853.7	
$C_4H_8N_2O_3$	*L*-Asparagine	929	891.5	
$C_4H_8N_2O_3$	*N*-Glycylglycine		882	
C_4H_8O	Ethyl vinyl ether	870.1	840.4	
C_4H_8O	2-Methoxy-1-propene	894.9	866.1	
C_4H_8O	Butanal	792.7	760.8	
C_4H_8O	Isobutanal	797.3	765.5	
C_4H_8O	2-Butanone	827.3	795.5	
C_4H_8O	Tetrahydrofuran	822.1	794.7	
$C_4H_8O_2$	Propyl formate	804.9	773.9	
$C_4H_8O_2$	Isopropyl formate	811.3	780.3	
$C_4H_8O_2$	Ethyl acetate	835.7	804.7	
$C_4H_8O_2$	Methyl propanoate	830.2	799.2	
$C_4H_8O_2$	1,3-Dioxane	825.4	796.2	
$C_4H_8O_2$	1,4-Dioxane	797.4	770.0	
$C_4H_8O_3$	Ethyl methyl carbonate	842.7	810.8	
C_4H_8S	Tetrahydrothiophene	849.1	819.3	
C_4H_9N	Pyrrolidine	948.3	915.3	
C_4H_9NO	*N*-Methylpropanamide	920.4	889.4	
C_4H_9NO	2-Methylpropanamide	878.6	846.7	
C_4H_9NO	*N*-Ethylacetamide	898.0	867.0	
C_4H_9NO	*N,N*-Dimethylacetamide	908.0	877.0	
C_4H_9NO	Morpholine	924.3	891.2	
$C_4H_9NO_2$	*tert*-Butyl nitrite	863.9	831.4	
$C_4H_9NO_2$	Ethyl *N*-methylcarbamate	888.8	857.8	
$C_4H_9NO_3$	*L*-Threonine	922.5	888.5	
C_4H_9NS	*N,N*-Dimethylthioacetamide	925.3	894.4	
C_4H_{10}	Isobutane	677.8	671.3	
$C_4H_{10}N_2$	Piperazine	943.7	914.7	
$C_4H_{10}N_2$	3-Ethyl-3-methyldiaziridine	903.8	871.3	
$C_4H_{10}O$	1-Butanol	789.2	758.9	
$C_4H_{10}O$	2-Butanol	815.7	784.6	
$C_4H_{10}O$	2-Methyl-1-propanol	793.7	762.2	
$C_4H_{10}O$	2-Methyl-2-propanol	802.6	772.2	
$C_4H_{10}O$	Diethyl ether	828.4	801	
$C_4H_{10}O$	Methyl propyl ether	814.9	785.7	
$C_4H_{10}O$	Isopropyl methyl ether	826.3	797.1	
$C_4H_{10}O_2$	1,4-Butanediol	915.6	854.9	
$C_4H_{10}O_2$	1,2-Dimethoxyethane	858.0	820.2	
$C_4H_{10}O_3$	1,2,4-Butanetriol	905.9	841	
$C_4H_{10}S$	1-Butanethiol	801.7	770.5	
$C_4H_{10}S$	2-Methyl-1-propanethiol	802.6	771.4	
$C_4H_{10}S$	2-Methyl-2-propanethiol	816.4	785.1	
$C_4H_{10}S$	Diethyl sulfide	856.7	827.0	
$C_4H_{11}N$	Butylamine	921.5	886.6	
$C_4H_{11}N$	*tert*-Butylamine	934.1	899.9	
$C_4H_{11}N$	Isobutylamine	924.8	890.8	
$C_4H_{11}N$	Diethylamine	952.4	919.4	
$C_4H_{11}N$	Isopropylmethylamine	952.4	919.4	
$C_4H_{11}N$	Ethyldimethylamine	960.1	929.1	
$C_4H_{11}NO$	*N*-Ethyl-*N*-hydroxyethanamine	914.7	882.2	
$C_4H_{11}NO$	4-Amino-1-butanol	984.5	932.1	
$C_4H_{11}NO_2$	Diethanolamine	953	920	
$C_4H_{12}N_2$	1,4-Butanediamine	1005.6	954.3	
$C_4H_{12}N_2$	*N,N'*-Dimethyl-1,2-ethanediamine	989.2	946.9	
$C_4H_{12}Sn$	Tetramethylstannane	823.7	797.4	

Molecular formula	Name	E_{pa} kJ/mol	$\Delta_{base}G°$ kJ/mol	Notes
$C_4H_{14}OSi_2$	1,1,3,3-Tetramethyldisiloxane	845.3	814.6	
C_4NiO_4	Nickel carbonyl	742.3	716.0	
C_5F_5N	Perfluoropyridine	764.9	733.0	
C_5FeO_5	Iron pentacarbonyl	833.0	798.5	
$C_5H_3ClN_4$	6-Chloro-1*H*-purine	873.6	841.7	
C_5H_4BrN	2-Bromopyridine	904.8	873.0	
C_5H_4BrN	3-Bromopyridine	910.0	878.2	
C_5H_4BrN	4-Bromopyridine	917.8	886.0	
C_5H_4ClN	2-Chloropyridine	900.9	869	
C_5H_4ClN	3-Chloropyridine	903.4	871.5	
C_5H_4ClN	4-Chloropyridine	916.1	884.2	
C_5H_4FN	3-Fluoropyridine	902.0	870.1	
C_5H_4FN	2-Fluoropyridine	884.6	852.7	
$C_5H_4N_2O_2$	4-Nitropyridine	874.3	842.5	
$C_5H_4N_2O_3$	4-Nitropyridine 1-oxide	868.0	837.3	
$C_5H_4N_4$	1*H*-Purine	920.1	888.2	
$C_5H_4N_4O$	Hypoxanthine	912.3	880.5	
C_5H_5	Cyclopentadienyl	831.5	799.1	
C_5H_5N	Pyridine	930	898.1	
C_5H_5NO	3-Pyridinol	929.5	897.7	
C_5H_5NO	Pyridine-1-oxide	923.6	892.9	
$C_5H_5N_5$	Adenine	942.8	912.5	
$C_5H_5N_5O$	Guanine	959.5	927.6	
C_5H_6	1,3-Cyclopentadiene	821.6	798.4	
$C_5H_6N_2$	2-Pyridinamine	947.2	915.3	
$C_5H_6N_2$	3-Pyridinamine	954.4	922.6	
$C_5H_6N_2$	4-Pyridinamine	979.7	947.8	
$C_5H_6N_2O_2$	Thymine	880.9	850.0	
C_5H_6O	2-Methylfuran	865.9	833.5	
C_5H_6O	3-Methylfuran	854.0	821.5	
$C_5H_6O_3$	Glutaric anhydride	816		Ref. 9
$C_5H_6O_3$	3-Methylsuccinic anhydride	807		Ref. 9
C_5H_6S	2-Methylthiophene	859.0	826.5	
$C_5H_7F_3O_2$	Propyl trifluoroacetate	763.9	732.9	
C_5H_8	*trans*-1,3-Pentadiene	834.1	804.4	
C_5H_8	2-Methyl-1,3-butadiene	826.4	797.6	
C_5H_8	2-Pentyne	810.2	778.0	
C_5H_8	3-Methyl-1-butyne	814.9	787.8	
C_5H_8	Cyclopentene	766.3	733.8	
C_5H_8	1-Methylcyclobutene	841.5	807.3	
C_5H_8	Vinylcyclopropane	816.3	787.5	
C_5H_8	3,3-Dimethylcyclopropene	847.8	817.1	
$C_5H_8N_2$	1,3-Dimethyl-1*H*-pyrazole	933.9	902.3	
$C_5H_8N_2$	1,4-Dimethyl-1*H*-imidazole	976.7	944.9	
$C_5H_8N_2$	1,5-Dimethyl-1*H*-pyrazole	934.3	902.8	
$C_5H_8N_2$	3,4-Dimethyl-1*H*-pyrazole	927.3	895.4	
$C_5H_8N_2$	3,5-Dimethyl-1*H*-pyrazole	933.5	900.1	
$C_5H_8N_2$	1,2-Dimethyl-1*H*-imidazole	984.7	952.6	
$C_5H_8N_2$	1,5-Dimethyl-1*H*-imidazole	977.6	945.8	
C_5H_8O	*trans*-2-Pentenal	839.0	807.2	
C_5H_8O	3-Methyl-2-butenal	856.9	825.0	
C_5H_8O	3-Methyl-3-buten-2-one	843.1	811.3	
C_5H_8O	Cyclopropyl methyl ketone	854.9	823	
C_5H_8O	Cyclopentanone	823.7	794.0	
C_5H_8O	3,4-Dihydro-2H-pyran	865.8	833.4	
$C_5H_8O_2$	3-Methyl-2-butenoic acid	822.9	791.9	
$C_5H_8O_2$	*cis*-2-Methyl-2-butenoic acid	822.5	791.5	
$C_5H_8O_2$	Cyclobutanecarboxylic acid	817.4	786.4	
$C_5H_8O_2$	Methyl trans-2-butenoate	851.3	820.4	
$C_5H_8O_2$	Methyl methacrylate	831.4	800.5	

Molecular formula	Name	E_{pa} kJ/mol	$\Delta_{base}G°$ kJ/mol	Notes
$C_5H_8O_2$	Methyl cyclopropanecarboxylate	842.1	811.2	
$C_5H_8O_2$	2,4-Pentanedione	873.5	836.8	
C_5H_9N	2-Isocyano-2-methylpropane	870.7	838.3	
C_5H_9N	3-(Dimethylamino)-1-propyne	940.3	909.5	
C_5H_9N	Pentanenitrile	802.4	771.7	
C_5H_9N	2,2-Dimethylpropanenitrile	810.9	780.2	
C_5H_9NO	3-Ethoxypropanenitrile	807.2	776.5	
C_5H_9NO	*N,N*-Dimethyl-2-propenamide	904.3	873.4	
C_5H_9NO	*N*-Methyl-2-pyrrolidone	923.5	891.6	
$C_5H_9NO_2$	*L*-Proline	920.5	886.0	
$C_5H_9NO_4$	*L*-Glutamic acid	913.0	879.1	
$C_5H_9N_3$	Histamine	999.8	961.9	
C_5H_{10}	2-Methyl-2-butene	808.8	779.9	
$C_5H_{10}N_2O$	1,3-Dimethyl-2-imidazolidinone	918.4	886.0	
$C_5H_{10}N_2O_3$	*L*-Glutamine	937.8	900	
$C_5H_{10}O$	Allyl ethyl ether	833.7	804.5	
$C_5H_{10}O$	Pentanal	796.6	764.8	
$C_5H_{10}O$	2-Pentanone	832.7	800.9	
$C_5H_{10}O$	3-Pentanone	836.8	807	
$C_5H_{10}O$	3-Methyl-2-butanone	836.3	804.4	
$C_5H_{10}O$	Tetrahydropyran	822.8	795.4	
$C_5H_{10}O$	2-Methyltetrahydrofuran	840.8	811.6	
$C_5H_{10}O_2$	Butyl formate	806.0	775	
$C_5H_{10}O_2$	Propyl acetate	836.6	805.6	
$C_5H_{10}O_2$	Isopropyl acetate	836.6	805.6	
$C_5H_{10}O_2$	Methyl butanoate	836.4	805.4	
$C_5H_{10}O_2$	Methyl isobutanoate	836.6	805.7	
$C_5H_{10}O_2$	*cis*-1,2-Cyclopentanediol	885.6	853.1	
$C_5H_{10}S$	Thiacyclohexane	855.8	826.0	
$C_5H_{11}N$	Allyldimethylamine	957.8	926.8	
$C_5H_{11}N$	Piperidine	954.0	921	
$C_5H_{11}N$	*N*-Methylpyrrolidine	965.6	934.8	
$C_5H_{11}NO$	2,2-Dimethylpropanamide	889.0	857.2	
$C_5H_{11}NO_2$	*L*-Valine	910.6	876.7	
$C_5H_{11}NO_2S$	*L*-Methionine	935.4	901.5	
$C_5H_{12}N_2O$	Tetramethylurea	930.6	899.6	
$C_5H_{12}N_2S$	Tetramethylthiourea	947.6	916.6	
$C_5H_{12}O$	2,2-Dimethyl-1-propanol	795.5	765.2	
$C_5H_{12}O$	Butyl methyl ether	820.3	791.2	
$C_5H_{12}O$	Methyl tert-butyl ether	841.6	812.4	
$C_5H_{12}O$	Ethyl isopropyl ether	842.7	813.5	
$C_5H_{12}S$	2,2-Dimethyl-1-propanethiol	809.5	778.2	
$C_5H_{12}Si$	Vinyltrimethylsilane	833	804.1	
$C_5H_{13}N$	Pentylamine	923.5	889.5	
$C_5H_{13}N$	2-Methyl-2-butanamine	937.8	903.6	
$C_5H_{13}N$	2,2-Dimethylpropylamine	928.3	894.0	
$C_5H_{13}N$	Ethylisopropylamine	960.0	926.7	
$C_5H_{13}N$	*N,N*-Dimethyl-1-propanamine	962.8	931.9	
$C_5H_{13}N$	Diethylmethylamine	971.0	940.0	
$C_5H_{13}N_3$	1,1,3,3-Tetramethylguanidine	1031.6	997.4	
$C_5H_{14}N_2$	*N,N,N′,N′*-Tetramethylmethanediamine	952.2	919.8	
$C_5H_{14}N_2$	*N,N*-Dimethyl-1,3-propanediamine	1025.0	975.3	
$C_5H_{14}N_2$	1,5-Pentanediamine	999.6	946.2	
C_6CrO_6	Chromium carbonyl	739.2	714.6	
C_6F_6	Hexafluorobenzene	648.0	624.4	
C_6HF_5	Pentafluorobenzene	690.4	662.7	
$C_6H_2F_4$	1,2,3,4-Tetrafluorobenzene	700.4	672.7	
$C_6H_2F_4$	1,2,3,5-Tetrafluorobenzene	747.3	719.6	
$C_6H_2F_4$	1,2,4,5-Tetrafluorobenzene	746.5	718.8	
$C_6H_3F_3$	1,2,3-Trifluorobenzene	724.3	696.6	

Molecular formula	Name	E_{pa} kJ/mol	$\Delta_{base}G°$ kJ/mol	Notes
$C_6H_3F_3$	1,2,4-Trifluorobenzene	729.5	699.4	
$C_6H_3F_3$	1,3,5-Trifluorobenzene	741.9	715.4	
C_6H_4	Benzyne	841	808.5	
$C_6H_4F_2$	*o*-Difluorobenzene	731.2	703.5	
$C_6H_4F_2$	*m*-Difluorobenzene	749.7	722	
$C_6H_4F_2$	*p*-Difluorobenzene	718.7	692.8	
$C_6H_4N_2$	2-Pyridinecarbonitrile	872.9	841	
$C_6H_4N_2$	3-Pyridinecarbonitrile	877.0	845.1	
$C_6H_4N_2$	4-Pyridinecarbonitrile	880.6	848.8	
$C_6H_4O_2$	*p*-Benzoquinone	799.1	769.3	
C_6H_5	Phenyl	884	851.5	
C_6H_5Br	Bromobenzene	754.1	725.8	
C_6H_5Cl	Chlorobenzene	753.1	724.6	
C_6H_5F	Fluorobenzene	755.9	726.6	
C_6H_5NO	Nitrosobenzene	854.3	823.6	
C_6H_5NO	4-Pyridinecarboxaldehyde	904.6	872.8	
$C_6H_5NO_2$	Nitrobenzene	800.3	769.5	
$C_6H_5N_3$	Azidobenzene	820	787.5	
C_6H_5O	Phenoxy	873.2		Ref. 4
C_6H_6	Benzene	750.4	725.4	
C_6H_6BrN	3-Bromoaniline	873.2	841.4	
C_6H_6ClN	3-Chloroaniline	868.1	836.3	
C_6H_6ClN	4-Chloroaniline	873.8	842.0	
C_6H_6ClN	2-Chloro-4-methylpyridine	921.2	889.4	
C_6H_6ClN	2-Chloro-6-methylpyridine	908.0	876.2	
C_6H_6ClNO	2-Chloro-6-methoxypyridine	909.9	878.0	
C_6H_6FN	3-Fluoroaniline	867.3	835.5	
C_6H_6FN	4-Fluoroaniline	871.5	839.7	
C_6H_6IN	3-Iodoaniline	878.7	846.8	
C_6H_6N	Anilino	949.8	917.4	
$C_6H_6N_2O$	3-Pyridinecarboxamide	918.3	886.4	
$C_6H_6N_2O_2$	4-Nitroaniline	866.0	834.2	
$C_6H_6N_4$	6-Methyl-1*H*-purine	939.2	907.3	
C_6H_6O	Bis(2-propynyl) ether	783.9	756.5	
C_6H_6O	Phenol	817.3	786.3	
C_6H_7N	Bis(2-propynyl)amine	910.0	876.9	
C_6H_7N	Aniline	882.5	850.6	
C_6H_7N	2-Methylpyridine	949.1	917.3	
C_6H_7N	3-Methylpyridine	943.4	911.6	
C_6H_7N	4-Methylpyridine	947.2	915.3	
C_6H_7NO	1-Methyl-2(1*H*)-pyridinone	925.8	894.8	
C_6H_7NO	2-Aminophenol	898.8	866.9	
C_6H_7NO	3-Aminophenol	898.8	866.9	
C_6H_7NO	2-Methoxypyridine	934.7	902.8	
C_6H_7NO	3-Methoxypyridine	942.7	910.9	
C_6H_7NO	4-Methoxypyridine	961.7	929.8	
C_6H_7NO	3-Methylpyridine-1-oxide	935.2	902.8	
C_6H_8	1,3-Cyclohexadiene	837	804.5	
C_6H_8	1,4-Cyclohexadiene	837	808.0	
$C_6H_8N_2$	1,2-Benzenediamine	896.5	865.8	
$C_6H_8N_2$	1,3-Benzenediamine	929.9	899.2	
$C_6H_8N_2$	1,4-Benzenediamine	905.9	874.0	
$C_6H_8N_2O$	Bis(2-cyanoethyl) ether	813.8	786.4	
C_6H_8O	2,4-Dimethylfuran	894.7	862.3	
C_6H_8O	2,5-Dimethylfuran	865.9	835.2	
C_6H_8O	3,4-Dimethylfuran	869.0	838.3	
$C_6H_8O_2$	1,3-Cyclohexanedione	881.2	849.4	
$C_6H_8O_2$	1,4-Cyclohexanedione	812.5	782.7	
$C_6H_8O_2$	1,2-Cyclohexanedione	849.6	818.9	
$C_6H_8O_3$	4-Methylglutaric anhydride	820		Ref. 9

Molecular formula	Name	E_{pa} kJ/mol	$\Delta_{base}G°$ kJ/mol	Notes
$C_6H_9F_3O_2$	Butyl trifluoroacetate	764.8	733.8	
C_6H_9N	2,5-Dimethylpyrrole	918.7	887.1	
$C_6H_9N_3O_2$	*L*-Histidine	988	950.2	
C_6H_{10}	Methylenecyclopentane	832.4	803.5	
C_6H_{10}	(1-Methylvinyl)cyclopropane	871.6	842.7	
C_6H_{10}	2-Methyl-1,3-pentadiene	864.9	836	
C_6H_{10}	3-Methyl-1,3-pentadiene	852.3	823.4	
C_6H_{10}	2,3-Dimethyl-1,3-butadiene	835.0	807.8	
C_6H_{10}	1-Hexyne	799.8	774.8	
C_6H_{10}	2-Hexyne	806.1	781.1	
C_6H_{10}	Cyclohexene	784.5	752.0	
C_6H_{10}	1-Methylcyclopentene	816.5	787.1	
$C_6H_{10}N_2$	1,3,5-Trimethyl-1*H*-pyrazole	949.3	917.4	
$C_6H_{10}N_2$	3,4,5-Trimethyl-1*H*-pyrazole	949.3	916.0	
$C_6H_{10}O$	7-Oxabicyclo[2.2.1]heptane	844.2	816.8	
$C_6H_{10}O$	7-Oxabicyclo[4.1.0]heptane	848.1	815.6	
$C_6H_{10}O$	*trans*-3-Hexen-2-one	865.6	833.8	
$C_6H_{10}O$	Diallyl ether	827.4	800.0	
$C_6H_{10}O$	Cyclohexanone	841.0	811.2	
$C_6H_{10}O$	Mesityl oxide	878.7	846.9	
$C_6H_{10}O_2$	Cyclopentanecarboxylic acid	817.4	786.4	
$C_6H_{10}O_2$	2,5-Hexanedione	892.0	851.8	
$C_6H_{11}N$	*N*-Allyl-2-propen-1-amine	949.3	916.3	
$C_6H_{11}NO$	1-Methyl-2-piperidinone	924.4	892.6	
$C_6H_{11}N_3O_4$	*N*-(*N*-Glycylglycyl)glycine	966.8	916.8	
C_6H_{12}	1-Hexene	805.2	776.3	
C_6H_{12}	2-Methyl-2-pentene	812	783.1	
C_6H_{12}	2,3-Dimethyl-2-butene	813.9	785.9	
C_6H_{12}	Cyclohexane	686.9	666.9	
$C_6H_{12}N_2$	Triethylenediamine	963.4	934.6	
$C_6H_{12}N_2O_3$	*N*-*L*-Alanyl-*L*-alanine		905.6	
$C_6H_{12}O$	Oxepane	834.2	806.8	
$C_6H_{12}O$	3-Hexanone	843.2	811.3	
$C_6H_{12}O$	3,3-Dimethyl-2-butanone	840.1	808.2	
$C_6H_{12}O_2$	*cis*-1,3-Cyclohexanediol	882.2	849.7	
$C_6H_{12}O_2$	*trans*-1,3-Cyclohexanediol	828.6	797.9	
$C_6H_{12}O_2$	Methyl 2,2-dimethylpropanoate	845.2	814.2	
$C_6H_{12}O_2$	Diacetone alcohol	822.9	791.1	
$C_6H_{12}O_6$	α-*D*-Glucose		778.9	
$C_6H_{12}O_6$	β-*D*-Glucose		778.9	
$C_6H_{13}N$	*N*,*N*,2-Trimethylpropenylamine	967.0	934.5	
$C_6H_{13}N$	Cyclohexylamine	934.4	899.6	
$C_6H_{13}N$	1-Methylpiperidine	971.1	940.1	
$C_6H_{13}N$	Hexahydro-1*H*-azepine	956.7	923.5	
$C_6H_{13}NO$	*N*,*N*-Dimethylbutanamide	921.7	890.8	
$C_6H_{13}NO$	*N*,*N*-Diethylacetamide	925.4	894.4	
$C_6H_{13}NO_2$	*L*-Leucine	914.6	880.6	
$C_6H_{13}NO_2$	*L*-Isoleucine	917.4	883.5	
$C_6H_{14}N_2O_2$	*L*-Lysine	996	951.0	
$C_6H_{14}N_4O_2$	*L*-Arginine	1051.0	1006.6	
$C_6H_{14}O$	Dipropyl ether	837.9	810.5	
$C_6H_{14}O$	Diisopropyl ether	855.5	828.1	
$C_6H_{14}O$	*tert*-Butyl ethyl ether	856.0	826.9	
$C_6H_{14}O_3$	Diethylene glycol dimethyl ether	918.8	870.9	
$C_6H_{14}S$	Dipropyl sulfide	864.7	834.9	
$C_6H_{14}S$	Diisopropyl sulfide	876.4	846.6	
$C_6H_{15}N$	Butyldimethylamine	969.2	938.2	
$C_6H_{15}N$	Isobutyldimethylamine	968.7	937.8	
$C_6H_{15}N$	Hexylamine	927.5	893.5	
$C_6H_{15}N$	Dipropylamine	962.3	929.3	

Molecular formula	Name	E_{pa} kJ/mol	$\Delta_{base}G°$ kJ/mol	Notes
$C_6H_{15}N$	Diisopropylamine	971.9	938.6	
$C_6H_{15}N$	Triethylamine	981.8	951	
$C_6H_{15}NO$	6-Amino-1-hexanol	969.0	915.7	
$C_6H_{15}OP$	Triethylphosphine oxide	936.6	906.8	
$C_6H_{15}O_4P$	Triethyl phosphate	909.3	879.6	
$C_6H_{15}P$	Triethylphosphine	984.5	952.0	
$C_6H_{16}N_2$	1,6-Hexanediamine	999.5	946.2	
$C_6H_{16}N_2$	*N,N,N′,N′*-Tetramethyl-1,2-ethanediamine	1012.8	970.6	
$C_6H_{16}OSi$	Triethylsilanol	822.1	794.8	
$C_6H_{18}N_3OP$	Hexamethylphosphoric triamide	958.6	928.7	
$C_6H_{18}N_3P$	Hexamethylphosphorous triamide	930.1	897.7	
$C_6H_{18}OSi_2$	Hexamethyldisiloxane	846.4	816.2	
C_6MoO_6	Molybdenum hexacarbonyl	762.6	738.1	
C_6O_6W	Tungsten carbonyl	758.0	733.4	
$C_7H_4N_2O_2$	3-Nitrobenzonitrile	781.4	750.7	
$C_7H_4N_2O_2$	4-Nitrobenzonitrile	775.7	745.1	
C_7H_5ClO	3-Chlorobenzaldehyde	813.0	781.1	
C_7H_5ClO	4-Chlorobenzaldehyde	831.3	799.4	
C_7H_5FO	3-Fluorobenzaldehyde	814.3	782.5	
C_7H_5FO	4-Fluorobenzaldehyde	827.1	795.3	
C_7H_5N	Benzonitrile	811.5	780.9	
C_7H_5N	Isocyanobenzene	868.4	836.0	
C_7H_5NO	Benzoxazole	891.6	859.8	
$C_7H_5NO_3$	4-Nitrobenzaldehyde	795.1	763.2	
C_7H_6ClNO	3-Chlorobenzamide	877.2	846.3	
C_7H_6ClNO	4-Chlorobenzamide	877.2	846.3	
C_7H_6F	*m*-Fluorobenzyl	836.5	804	
C_7H_6FNO	3-Fluorobenzamide	877.2	846.3	
C_7H_6FNO	4-Fluorobenzamide	877.2	846.3	
$C_7H_6F_3N$	3-(Trifluoromethyl)aniline	856.9	825.1	
$C_7H_6N_2$	1*H*-Benzimidazole	953.8	920.5	
$C_7H_6N_2$	1*H*-Indazole	900.8	868.9	
$C_7H_6N_2$	3-Aminobenzonitrile	842.3	810.4	
$C_7H_6N_2$	1*H*-Pyrrolo[2,3-b]pyridine	940.2	908.3	
$C_7H_6N_2O_3$	4-Nitrobenzamide	845.3	814.4	
$C_7H_6N_2O_3$	3-Nitrobenzamide	854.2	823.2	
C_7H_6O	Benzaldehyde	834.0	802.1	
C_7H_6O	2,4,6-Cycloheptatrien-1-one	920.8	891.0	
$C_7H_6O_2$	Benzoic acid	821.1	790.1	
C_7H_7	Benzyl	831.4	800.7	
C_7H_7Br	2-Bromotoluene	775.3	745.8	
C_7H_7Br	3-Bromotoluene	782.0	752.5	
C_7H_7Br	4-Bromotoluene	775.3	745.8	
C_7H_7Cl	2-Chlorotoluene	790.5	761.1	
C_7H_7Cl	3-Chlorotoluene	783.9	754.5	
C_7H_7Cl	4-Chlorotoluene	762.9	735.2	
C_7H_7F	2-Fluorotoluene	773.3	743.8	
C_7H_7F	3-Fluorotoluene	785.4	756.0	
C_7H_7F	4-Fluorotoluene	763.8	736.1	
C_7H_7I	1-Iodo-2-methylbenzene	780.3	750.8	
C_7H_7N	4-Vinylpyridine	944.1	912.3	
C_7H_7NO	1-(3-Pyridinyl)ethanone	916.2	884.3	
C_7H_7NO	1-(4-Pyridinyl)ethanone	914.7	882.9	
C_7H_7NO	4-Aminobenzaldehyde	910.4	878.6	
C_7H_7NO	Benzamide	892.1	861.2	
$C_7H_7NO_2$	Methyl 3-pyridinecarboxylate	925.6	893.8	
$C_7H_7NO_2$	Methyl 4-pyridinecarboxylate	926.6	894.7	
$C_7H_7NO_2$	Aniline-2-carboxylic acid	901.5	869.0	
$C_7H_7NO_2$	Aniline-3-carboxylic acid	864.7	832.3	

Molecular formula	Name	E_{pa} kJ/mol	$\Delta_{base}G°$ kJ/mol	Notes
$C_7H_7NO_2$	Aniline-4-carboxylic acid	864.7	832.3	
$C_7H_7NO_2$	4-Nitrotoluene	815.2	782.7	
$C_7H_7NO_3$	4-Nitrobenzenemethanol	810.5	778.0	
$C_7H_7N_3$	1-Methyl-1*H*-benzotriazole	931.2	898.7	
C_7H_7O	2-Methylphenoxy	874.5	842	
C_7H_8	Toluene	784.0	756.3	
C_7H_8	2,5-Norbornadiene	849.3	820.3	
$C_7H_8N_2O$	4-Aminobenzamide	927.9	896.9	
$C_7H_8N_2O$	3-Aminobenzamide	900.9	869.9	
$C_7H_8N_2O_2$	*N*-Methyl-4-nitroaniline	891.6	865.1	
C_7H_8O	*o*-Cresol	832	800	Ref. 10
C_7H_8O	*m*-Cresol	841	809	Ref. 10
C_7H_8O	*p*-Cresol	814	782	Ref. 10
C_7H_8O	Benzyl alcohol	778.3	748.0	
C_7H_8O	Anisole	839.6	807.2	
$C_7H_8O_2$	2,6-Dimethyl-4*H*-pyran-4-one	941.5	907.3	
$C_7H_8O_2S$	Methyl phenyl sulfone	812.7	780.3	
C_7H_8S	(Methylthio)benzene	872.6	843.7	
C_7H_9N	Benzylamine	913.3	879.4	
C_7H_9N	2-Methylaniline	890.9	859.1	
C_7H_9N	3-Methylaniline	895.8	864.0	
C_7H_9N	4-Methylaniline	896.7	864.8	
C_7H_9N	*N*-Methylaniline	916.6	890.1	
C_7H_9N	2-Ethylpyridine	952.4	920.6	
C_7H_9N	3-Ethylpyridine	947.4	915.5	
C_7H_9N	4-Ethylpyridine	951.1	919.2	
C_7H_9N	2,3-Dimethylpyridine	958.9	927.0	
C_7H_9N	2,4-Dimethylpyridine	962.9	930.8	
C_7H_9N	2,5-Dimethylpyridine	958.8	926.9	
C_7H_9N	2,6-Dimethylpyridine	963.0	931.1	
C_7H_9N	3,4-Dimethylpyridine	957.3	925.5	
C_7H_9N	3,5-Dimethylpyridine	955.4	923.5	
C_7H_9NO	2-Methoxyaniline	905.2	873.3	
C_7H_9NO	3-Methoxyaniline	913.0	881.1	
C_7H_9NO	4-Methoxyaniline	900.3	868.5	
C_7H_{10}	Bicyclo[2.2.1]hept-2-ene	836.5	804.0	
$C_7H_{10}N_2$	*N,N*-Dimethyl-2-pyridinamine	968.2	941.6	
$C_7H_{10}N_2$	*N,N*-Dimethyl-4-pyridinamine	997.6	971.1	
$C_7H_{10}O$	Dicyclopropyl ketone	880.4	850.6	
$C_7H_{10}O$	Bicyclo[2.2.1]heptan-2-one	847.4	815.5	
$C_7H_{11}N$	Cyclohexanecarbonitrile	815.0	784.4	
C_7H_{12}	2,4-Dimethyl-1,3-pentadiene	886.5	857.6	
C_7H_{12}	1-Methylcyclohexene	825.1	792.6	
C_7H_{12}	1,2-Dimethylcyclopentene	822.6	791.9	
$C_7H_{12}N_2$	2,3,4,6,7,8-Hexahydropyrrolo[1,2-a]pyrimidine	1038.3	1005.9	
$C_7H_{12}O$	Cycloheptanone	845.6	815.9	
$C_7H_{12}O$	4-Methylcyclohexanone	844.9	813.0	
$C_7H_{12}O_2$	Cyclohexanecarboxylic acid	823.8	792.8	
$C_7H_{13}N$	1-Azabicyclo[2.2.2]octane	983.3	952.5	
C_7H_{14}	2,4-Dimethyl-2-pentene	812	783.1	
$C_7H_{14}O$	Methoxycyclohexane	840.5	811.3	
$C_7H_{14}O$	4-Heptanone	845.0	815.3	
$C_7H_{14}O$	2,4-Dimethyl-3-pentanone	850.3	820.5	
$C_7H_{14}O$	Cyclohexanemethanol	802.1	771.7	
$C_7H_{15}N$	Cyclohexanemethanamine	926.6	895.8	
$C_7H_{16}O$	*tert*-Butyl isopropyl ether	870.7	841.5	
$C_7H_{17}N$	Heptylamine	923.2	889.3	
$C_7H_{17}N$	Methyldipropylamine	983.5	950.9	
$C_7H_{17}N$	Diethylpropylamine	978.8	947.9	

Molecular formula	Name	E_{pa} kJ/mol	$\Delta_{base}G°$ kJ/mol	Notes
$C_7H_{18}N_2$	1,7-Heptanediamine	998.5	944.9	
$C_7H_{18}N_2$	*N,N,N',N'*-Tetramethyl-1,3-propanediamine	1035.2	985.4	
$C_8H_4F_3N$	3-(Trifluoromethyl)benzonitrile	791.4	760.8	
$C_8H_4F_3N$	4-(Trifluoromethyl)benzonitrile	787.2	758.3	
$C_8H_4N_2$	*m*-Dicyanobenzene	779.3	750.4	
$C_8H_4N_2$	*p*-Dicyanobenzene	779.0	751.8	
C_8H_5Cl	1-Chloro-4-ethynylbenzene	832.4	801.7	
$C_8H_5Cl_3O$	2,2,2-Trichloro-1-phenylethanone	818.9	787.0	
$C_8H_5F_3O$	2,2,2-Trifluoro-1-phenylethanone	799.2	767.4	
$C_8H_5F_3O$	4-(Trifluoromethyl)benzaldehyde	805.6	773.8	
C_8H_5NO	4-Formylbenzonitrile	796.9	766.3	
C_8H_6	Phenylacetylene	832.0	801.3	
C_8H_6ClN	4-(Chloromethyl)benzonitrile	812.8	782.1	
C_8H_6ClN	3-(Chloromethyl)benzonitrile	811.2	780.6	
$C_8H_6N_2$	Quinoxaline	903.8	873.7	
$C_8H_6N_2$	Cinnoline	936.3	904.4	
C_8H_7Br	1-Bromo-4-vinylbenzene	838.7	809.8	
C_8H_7Br	1-Bromo-3-vinylbenzene	822.4	793.5	
C_8H_7ClO	1-(3-Chlorophenyl)ethanone	846.9	815.1	
C_8H_7ClO	1-(4-Chlorophenyl)ethanone	856.6	824.8	
$C_8H_7ClO_2$	Methyl 4-chlorobenzoate	842.1	811.1	
$C_8H_7ClO_2$	Methyl 3-chlorobenzoate	835.4	804.4	
C_8H_7FO	1-(4-Fluorophenyl)ethanone	858.6	826.8	
C_8H_7N	Benzeneacetonitrile	805.5	774.8	
C_8H_7N	1*H*-Indole	933.4	901.9	
$C_8H_7NO_3$	1-(4-Nitrophenyl)ethanone	824.3	792.5	
$C_8H_7NO_3$	1-(3-Nitrophenyl)ethanone	826.0	794.1	
$C_8H_7NO_4$	Methyl 3-nitrobenzoate	815.7	784.7	
$C_8H_7NO_4$	Methyl 4-nitrobenzoate	813.2	782.3	
C_8H_8	Styrene	839.5	809.2	
$C_8H_8N_2$	1-Methyl-1*H*-benzimidazole	967.0	935.2	
$C_8H_8N_2$	2-Methyl-2*H*-indazole	941.4	909.6	
$C_8H_8N_2$	1-Methyl-1*H*-indazole	922.4	890.5	
C_8H_8O	3-Methylbenzaldehyde	840.0	808.1	
C_8H_8O	4-Methylbenzaldehyde	851.8	820.0	
C_8H_8O	Acetophenone	861.1	829.3	
$C_8H_8O_2$	*o*-Toluic acid	838.8	807.8	
$C_8H_8O_2$	*m*-Toluic acid	829.8	798.8	
$C_8H_8O_2$	*p*-Toluic acid	836.7	805.7	
$C_8H_8O_2$	Methyl benzoate	850.5	819.5	
$C_8H_8O_2$	3-Methoxybenzaldehyde	844.1	812.2	
$C_8H_8O_2$	4-Methoxybenzaldehyde	881.1	849.3	
$C_8H_8O_2$	1-(3-Hydroxyphenyl)ethanone	863.6	831.8	
$C_8H_8O_2$	1-(4-Hydroxyphenyl)ethanone	883.7	851.9	
$C_8H_8O_3$	Methyl 4-hydroxybenzoate	863.4	832.5	
$C_8H_8O_3$	Methyl 3-hydroxybenzoate	850.0	819.1	
C_8H_9N	2,3-Dihydro-1*H*-indole	957.1	926.3	
C_8H_9NO	3-Methylbenzamide	900.9	869.9	
C_8H_9NO	4-Methylbenzamide	900.9	869.9	
C_8H_9NO	1-(4-Aminophenyl)ethanone	908.8	877.0	
$C_8H_9NO_2$	3-Methoxybenzamide	900.9	869.9	
$C_8H_9NO_2$	2,4-Dimethyl-1-nitrobenzene	831.0	798.5	
$C_8H_9NO_2$	Methyl 4-aminobenzoate	883.9	853.0	
$C_8H_9NO_2$	4-Methoxybenzamide	900.3	869.4	
C_8H_{10}	Ethylbenzene	788.0	760.3	
C_8H_{10}	*o*-Xylene	796.0	768.3	
C_8H_{10}	*m*-Xylene	812.1	786.2	
C_8H_{10}	*p*-Xylene	794.4	766.8	
$C_8H_{10}ClN$	4-Chloro-*N,N*-dimethylaniline	922.9	896.4	

Molecular formula	Name	E_{pa} kJ/mol	$\Delta_{base}G°$ kJ/mol	Notes
$C_8H_{10}N_2O_2$	*N,N*-Dimethyl-4-nitroaniline	896.7	870.2	
$C_8H_{10}N_2O_2$	*N,N*-Dimethyl-3-nitroaniline	894.1	867.6	
$C_8H_{10}O$	Benzyl methyl ether	816.7	787.5	
$C_8H_{10}O$	2-Methylanisole	850	818	Ref. 10
$C_8H_{10}O$	3-Methylanisole	860	828	Ref. 10
$C_8H_{10}O$	4-Methylanisole	841	809	Ref. 10
$C_8H_{11}N$	4-Isopropylpyridine	955.7	923.8	
$C_8H_{11}N$	3-Ethylaniline	897.9	866.1	
$C_8H_{11}N$	*N*-Ethylaniline	924.8	892.9	
$C_8H_{11}N$	*N,N*-Dimethylaniline	941.1	909.2	
$C_8H_{11}N$	2,6-Dimethylaniline	901.7	869.8	
$C_8H_{11}N$	Benzeneethanamine	936.2	902.3	
$C_8H_{11}N$	2-Propylpyridine	955.7	923.8	
C_8H_{12}	2-Methyl-2-norbornene	845	812.5	
$C_8H_{12}N_2$	*N,N*-Dimethyl-1,4-benzenediamine	955.0	928.4	
$C_8H_{12}N_2O_2$	Ethyl 1,5-dimethyl-1*H*-pyrazole-3-carboxylate	933.4	901.5	
$C_8H_{14}O$	Cyclooctanone	849.4	819.6	
$C_8H_{14}O$	1-Cyclohexylethanone	841.4	809.5	
$C_8H_{14}O_2$	Methyl cyclohexanecarboxylate	846.2	815.3	
$C_8H_{16}O$	2,2,4-Trimethyl-3-pentanone	856.9	825.0	
$C_8H_{17}N$	Cyclohexyldimethylamine	983.6	952.6	
$C_8H_{18}O$	Dibutyl ether	845.7	818.3	
$C_8H_{18}O$	Di-*sec*-butyl ether	865.9	838.5	
$C_8H_{18}O$	Di-*tert*-butyl ether	887.4	860.0	
$C_8H_{18}O_4$	Triethylene glycol dimethyl ether	946.6	892.4	
$C_8H_{18}O_5$	Tetraethylene glycol		>910	
$C_8H_{18}S$	Dibutyl sulfide	871.8	842.1	
$C_8H_{18}S$	Di-*tert*-butyl sulfide	893.8	864.0	
$C_8H_{19}N$	*N*-Ethyl-*N*-isopropyl-2-propanamine	994.3	963.5	
$C_8H_{19}N$	Octylamine	928.9	895.0	
$C_8H_{19}N$	Dibutylamine	968.5	935.3	
$C_8H_{19}N$	Di-*sec*-butylamine	980.7	947.5	
$C_8H_{19}N$	Diisobutylamine	958.1	925.1	
$C_8H_{20}N_2$	*N,N,N',N'*-Tetramethyl-1,4-butanediamine	1046.3	992.7	
$C_8H_{20}N_2$	Tetraethylhydrazine	964.3	935.3	
$C_9H_7MnO_3$	Manganese 2-methylcyclopentadienyl tricarbonyl	833.8	801.3	
C_9H_7N	Quinoline	953.2	921.4	
C_9H_7N	Isoquinoline	951.7	919.9	
C_9H_7NO	4-Acetylbenzonitrile	826.8	795.0	
C_9H_8	Indene	848.8	819.6	
C_9H_8O	2-Methylbenzofuran	859.6	827.2	
$C_9H_8O_3$	Methyl 4-formylbenzoate	832.9	801.9	
C_9H_9Cl	1-Chloro-4-isopropenylbenzene	854.3	825.4	
$C_9H_9ClO_2$	3-Chloro-4-methoxyacetophenone	883.7	851.9	
C_9H_{10}	2-Methylstyrene	855.2	826.3	
C_9H_{10}	3-Methylstyrene	849.4	820.5	
C_9H_{10}	4-Methylstyrene	861.7	832.8	
C_9H_{10}	*cis*-1-Propenylbenzene	836.4	807.5	
C_9H_{10}	*trans*-1-Propenylbenzene	834.2	805.3	
C_9H_{10}	Isopropenylbenzene	864.2	835.3	
C_9H_{10}	Cyclopropylbenzene	834.9	802.4	
$C_9H_{10}N_2$	4-(Dimethylamino)benzonitrile	889.1	862.6	
$C_9H_{10}O$	1-(3-Methylphenyl)ethanone	868.2	836.4	
$C_9H_{10}O$	1-Phenyl-1-propanone	867.4	835.6	
$C_9H_{10}O$	1-Phenyl-2-propanone	842.6	810.8	
$C_9H_{10}O$	4-Methylacetophenone	875.5	843.6	
$C_9H_{10}OS$	4-Acetylthioanisole	888.2	856.3	
$C_9H_{10}O_2$	Methyl 2-methylbenzoate	858.3	827.3	

Molecular formula	Name	E_{pa} kJ/mol	$\Delta_{base}G°$ kJ/mol	Notes
$C_9H_{10}O_2$	Methyl 3-methylbenzoate	857.7	826.8	
$C_9H_{10}O_2$	1-(3-Methoxyphenyl)ethanone	871.2	839.3	
$C_9H_{10}O_2$	Methyl 4-methylbenzoate	861.5	830.6	
$C_9H_{10}O_2$	4-Acetylanisole	895.6	863.7	
$C_9H_{10}O_3$	Methyl 4-methoxybenzoate	870.6	839.6	
$C_9H_{10}O_3$	Methyl 3-methoxybenzoate	856.7	825.8	
$C_9H_{11}N$	5,6,7,8-Tetrahydroquinoline	966.0	934.1	
$C_9H_{11}N$	5,6,7,8-Tetrahydroisoquinoline	966.6	934.7	
$C_9H_{11}NO$	4-(Dimethylamino)benzaldehyde	924.8	898.3	
$C_9H_{11}NO$	*N,N*-Dimethylbenzamide	932.7	901.8	
$C_9H_{11}NO_2$	1,3,5-Trimethyl-2-nitrobenzene	823.8	793.1	
$C_9H_{11}NO_2$	*L*-Phenylalanine	922.9	888.9	
$C_9H_{11}NO_3$	*L*-Tyrosine	926	892.1	
C_9H_{12}	Propylbenzene	790.1	762.4	
C_9H_{12}	Isopropylbenzene	791.6	763.9	
C_9H_{12}	1,3,5-Trimethylbenzene	836.2	808.6	
$C_9H_{12}N_2$	3-(2-Pyrrolidinyl)pyridine, (*S*)-	964.0	931.0	
$C_9H_{12}N_2O_6$	Uridine	947.6	916.6	
$C_9H_{12}O_3$	1,3,5-Trimethoxybenzene	926.7	898.2	
$C_9H_{13}N$	*N*-Ethyl-*N*-methylaniline	939.0	912.4	
$C_9H_{13}N$	2,6-Diethylpyridine	972.3	940.4	
$C_9H_{13}N$	4-*tert*-Butylpyridine	957.7	925.8	
$C_9H_{13}N$	2-*tert*-Butylpyridine	961.7	929.8	
$C_9H_{13}N$	2-Methyl-*N,N*-dimethylaniline	951.8	925.3	
$C_9H_{13}N$	3-Methyl-*N,N*-dimethylaniline	942.1	915.7	
$C_9H_{13}N$	4-Methyl-*N,N*-dimethylaniline	950.0	918.1	
$C_9H_{13}N$	*N,N*-Dimethylbenzylamine	968.4	937.4	
$C_9H_{13}NO$	4-Methoxy-*N,N*-dimethylaniline	949.1	922.4	
$C_9H_{13}N_3O_5$	Cytidine	982.5	950.0	
$C_9H_{14}O$	Isophorone	893.5	861.6	
$C_9H_{15}N$	*N,N*-Diallyl-2-propen-1-amine	972.3	941.3	
$C_9H_{15}N$	*N*-(1-Cyclopenten-1-yl)pyrrolidine	1019.2	988.4	
$C_9H_{16}O$	Cyclononanone	852.6	822.8	
$C_9H_{17}N_3O_4$	*N*-(*N*-*L*-Alanyl-*L*-alanyl)-*L*-alanine		924.1	
$C_9H_{18}O$	5-Nonanone	853.7	821.9	
$C_9H_{18}O$	Di-*tert*-butyl ketone	861.3	831.5	
$C_9H_{19}N$	1-Isobutylpiperidine	974.5	943.5	
$C_9H_{19}N$	2,2,6,6-Tetramethylpiperidine	987.0	953.9	
$C_9H_{21}N$	Tripropylamine	991.0	960.1	
$C_{10}H_8$	Naphthalene	802.9	779.4	
$C_{10}H_8$	Azulene	925.2	896	
$C_{10}H_8N_2$	2,2'-Bipyridine	965		Ref. 7
$C_{10}H_9N$	1-Naphthylamine	907.0	875.1	
$C_{10}H_{10}Fe$	Ferrocene	863.6	841.3	
$C_{10}H_{10}N_2$	1,8-Naphthalenediamine	944.5	912.1	
$C_{10}H_{10}N_2$	1-Methyl-3-phenyl-1*H*-pyrazole	932.6	900.8	
$C_{10}H_{10}N_2$	1-Methyl-5-phenyl-1*H*-pyrazole	932.4	900.5	
$C_{10}H_{10}Ni$	Nickelocene	935.7	907.3	
$C_{10}H_{10}O_2$	1,4-Diacetylbenzene	850.8	821.0	
$C_{10}H_{10}O_2$	1,3-Diacetylbenzene	852.0	822.3	
$C_{10}H_{10}O_3$	4-Acetylphenyl acetate	853.2	821.3	
$C_{10}H_{10}O_4$	Dimethyl isophthalate	843.5	814.3	
$C_{10}H_{10}O_4$	Dimethyl terephthalate	843.2	812.3	
$C_{10}H_{10}Ru$	Ruthenocene	899.1	876.8	
$C_{10}H_{12}$	1-Methyl-3-(1-methylvinyl)benzene	867.6	838.7	
$C_{10}H_{12}$	1-Methyl-4-(1-methylvinyl)benzene	881.8	852.9	
$C_{10}H_{12}$	1-Methyl-2-(1-methylvinyl)benzene	857.8	828.9	
$C_{10}H_{12}$	1,2,3,4-Tetrahydronaphthalene	809.7	782.1	
$C_{10}H_{12}O$	1-(2,4-Dimethylphenyl)ethanone	882.6	850.8	
$C_{10}H_{12}O$	1-(2,5-Dimethylphenyl)ethanone	873.5	841.6	

Molecular formula	Name	E_{pa} kJ/mol	$\Delta_{base}G°$ kJ/mol	Notes
$C_{10}H_{12}O$	1-(3,4-Dimethylphenyl)ethanone	882.8	851.0	
$C_{10}H_{12}O_2$	Methyl 2,5-dimethylbenzoate	864.7	833.7	
$C_{10}H_{12}O_2$	Methyl 2,4-dimethylbenzoate	868.2	837.2	
$C_{10}H_{12}O_2$	Methyl 3,5-dimethylbenzoate	864.3	833.4	
$C_{10}H_{13}N$	1-Phenylpyrrolidine	941.6	915.1	
$C_{10}H_{13}NO$	4'-(Dimethylamino)acetophenone	932.8	906.3	
$C_{10}H_{13}NO$	*N,N*,3-Trimethylbenzamide	927.0	896.0	
$C_{10}H_{13}NO$	*N,N*,4-Trimethylbenzamide	927.0	896.0	
$C_{10}H_{13}NO$	1-[3-(Dimethylamino)phenyl]ethanone	928.0	901.5	
$C_{10}H_{13}N_5O_3$	2'-Deoxyadenosine	991.5	959.1	
$C_{10}H_{13}N_5O_4$	Adenosine	989.3	956.8	
$C_{10}H_{13}N_5O_5$	Guanosine	993.4	960.9	
$C_{10}H_{14}$	Butylbenzene	791.9	764.2	
$C_{10}H_{14}$	1,2,3,5-Tetramethylbenzene	845.6	816.5	
$C_{10}H_{14}ClN$	4-Chloro-*N,N*-diethylaniline	931.0	899.2	
$C_{10}H_{14}N_2$	*L*-Nicotine	963.4	932.6	
$C_{10}H_{14}N_2O$	*N,N*-Diethyl-3-pyridinecarboxamide	940.9	909.0	
$C_{10}H_{14}N_2O_5$	Thymidine	948.3	915.9	
$C_{10}H_{15}N$	*N,N*,2,6-Tetramethylaniline	954.1	923.2	
$C_{10}H_{15}N$	*N,N*,3,5-Tetramethylaniline	956.1	924.3	
$C_{10}H_{15}N$	*N,N*-Diethylaniline	959.8	927.9	
$C_{10}H_{16}N_2$	*N,N,N',N'*-Tetramethyl-1,2-benzenediamine	982.6	950.2	
$C_{10}H_{17}N$	Tricyclo[3.3.1.1^{3,7}]decan-1-amine	948.8	916.3	
$C_{10}H_{22}O$	Dipentyl ether	852.7	825.3	
$C_{10}H_{22}O_5$	Tetraethylene glycol dimethyl ether	953.8	897.8	
$C_{10}H_{23}N$	Decylamine	930.4	896.5	
$C_{10}H_{24}N_2$	*N,N,N',N'*-Tetramethyl-1,6-hexanediamine	1035.8	982.2	
$C_{11}H_9N$	4-Phenylpyridine	939.7	907.8	
$C_{11}H_{10}$	1-Methylnaphthalene	834.8	805.3	
$C_{11}H_{10}$	2-Methylnaphthalene	831.9	802.4	
$C_{11}H_{12}N_2O_2$	*L*-Tryptophan	948.9	915	
$C_{11}H_{14}O_2$	Methyl 2,4,6-trimethylbenzoate	866.3	835.3	
$C_{11}H_{15}N$	1-Phenylpiperidine	952.9	926.4	
$C_{11}H_{15}N$	Tricyclo[3.3.1.1^{3,7}]decane-1-carbonitrile	834.4	803.8	
$C_{11}H_{16}$	Pentamethylbenzene	850.7	823.5	
$C_{11}H_{17}N$	*N,N*-Diethyl-4-methylaniline	962.8	931.0	
$C_{11}H_{17}N$	2-Hexylpyridine	963.6	931.7	
$C_{11}H_{18}O$	1,4,7,7-Tetramethylbicyclo[2.2.1]heptan-2-one	863.3	831.4	
$C_{11}H_{24}O_4$	2,6,10,14-Tetraoxapentadecane		895.1	
$C_{12}H_8N_2$	Phenazine	938.4	908.3	
$C_{12}H_9NO$	Phenyl-3-pyridinylmethanone	934.1	902.3	
$C_{12}H_{10}$	Acenaphthene	851.7	821.0	
$C_{12}H_{10}$	Biphenyl	813.6	782.9	
$C_{12}H_{16}O$	1-(4-tert-Butylphenyl)ethanone	882.5	850.6	
$C_{12}H_{18}$	Hexamethylbenzene	860.6	836.0	
$C_{12}H_{18}O$	1-Tricyclo[3.3.1.1^{3,7}]dec-1-ylethanone	864.9	833.1	
$C_{12}H_{19}N$	*N,N*-Dipropylaniline	963.0	931.1	
$C_{12}H_{20}O$	2,5-Di-*tert*-butylfuran	894.7	863.9	
$C_{12}H_{27}N$	Tributylamine	998.5	967.6	
$C_{13}H_9N$	Acridine	972.6	940.7	
$C_{13}H_{10}$	9*H*-Fluorene	831.5	803.8	
$C_{13}H_{10}O$	Benzophenone	882.3	852.5	
$C_{13}H_{12}$	2-Methylbiphenyl	815.9	783.4	
$C_{13}H_{12}$	3-Methylbiphenyl	828.0	795.5	
$C_{13}H_{12}$	4-Methylbiphenyl	817.9	785.4	
$C_{13}H_{12}$	Diphenylmethane	802.0	769.5	
$C_{13}H_{13}P$	Methyldiphenylphosphine	972.1	939.7	

Molecular formula	Name	E_{pa} kJ/mol	$\Delta_{base}G°$ kJ/mol	Notes
$C_{13}H_{21}N$	2,6-Di-*tert*-butylpyridine	982.9	951	
$C_{13}H_{21}N$	2,4-Di-*tert*-butylpyridine	983.8	952.0	
$C_{13}H_{21}NO$	*N,N*-Dimethyltricyclo[3.3.1.1^{3,7}]decane-1-carboxamide	949.4	917.6	
$C_{14}H_{10}$	Anthracene	877.3	846.6	
$C_{14}H_{10}$	Phenanthrene	825.7	795.0	
$C_{14}H_{12}$	1,1-Diphenylethene	885.7	856.9	
$C_{14}H_{14}$	1,2-Diphenylethane	801.8	774.1	
$C_{14}H_{18}$	1,2,3,4,5,6,7,8-Octahydroanthracene	845.4	814.7	
$C_{14}H_{18}$	1,2,3,4,5,6,7,8-Octahydrophenanthrene	846.2	815.5	
$C_{14}H_{23}N$	4-Octylaniline	894.5	862	
$C_{15}H_{12}$	2-Methylanthracene	887.5	855.1	
$C_{15}H_{12}$	9-Methylanthracene	896.5	865.8	
$C_{15}H_{12}N_2$	3,5-Diphenyl-1*H*-pyrazole	946.3	912.7	
$C_{15}H_{16}$	1,3-Diphenylpropane	820.1	787.6	
$C_{15}H_{18}$	1,4-Dimethyl-7-isopropylazulene	983.1	950.6	
$C_{15}H_{24}$	1,3-Di-*tert*-butyl-5-methylbenzene	853.7	826.0	
$C_{16}H_{10}$	Fluoranthene	828.6	800.9	
$C_{16}H_{10}$	Pyrene	869.2	840.1	
$C_{16}H_{18}$	1,4-Diphenylbutane	822.0	779.8	
$C_{17}H_{20}$	1,5-Diphenylpentane	824.7	782.4	
$C_{18}H_{12}$	Chrysene	840.9	810.1	
$C_{18}H_{12}$	Naphthacene	905.5	876.5	
$C_{18}H_{12}$	Triphenylene	819.2	791.2	
$C_{18}H_{15}As$	Triphenylarsine	908.9	876.4	
$C_{18}H_{15}AsO$	Triphenylarsine oxide	906.2	876.4	
$C_{18}H_{15}N$	Triphenylamine	908.9	876.4	
$C_{18}H_{15}OP$	Triphenylphosphine oxide	906.2	876.4	
$C_{18}H_{15}P$	Triphenylphosphine	972.8	940.4	
$C_{18}H_{15}PS$	Triphenylphosphine sulfide	906.2	876.4	
$C_{18}H_{15}Sb$	Triphenylstibine	845.5	813.1	
$C_{18}H_{22}$	1,6-Diphenylhexane	826.1	783.8	
$C_{18}H_{30}$	1,3,5-Tri-*tert*-butylbenzene	848.8	822.3	
$C_{20}H_{12}$	Perylene	888.6	859.6	
$C_{22}H_{12}$	Benzo[ghi]perylene	876.0	845.2	
$C_{22}H_{14}$	Picene	851.3	820.6	
$C_{24}H_{12}$	Coronene	861.3	835.0	
C_{60}	Carbon (fullerene-C_{60})		827.5	
C_{70}	Carbon (fullerene-C_{70})		827.5	