

APPENDIX A. THERMODYNAMIC PARAMETERS

Table of Contents

APPENDIX A. THERMODYNAMIC PARAMETERS	A-1
A.1 Gas-phase entropy and enthalpy values.....	A-1
A.1 References.....	A-8

Tables

Table A-1. Gas-phase entropy and enthalpy values for selected species at 298.15 K and 100 kPa.	A-1
---	-----

A.1 Gas-phase entropy and enthalpy values

Table A-1 lists selected entropy and enthalpy of formation values at 298 K for a number of atmospheric species. As much as possible, the values were taken from primary evaluations, that is, evaluations that develop a recommended value from the original studies. Otherwise, the values were selected from the original literature, which is referenced in the table. Often, the enthalpy of formation and the entropy values are taken from different sources, usually due to a more recent value for the enthalpy of formation. The cited error limits are from the original references and therefore reflect often widely varying criteria. Some enthalpy values were corrected slightly to reflect the value of a reference compound selected for this table; these are indicated. Values that are calculated or estimated are also indicated in the table.

Table A-1. Gas-phase entropy and enthalpy values for selected species at 298.15 K and 100 kPa.

SPECIES	$\Delta H_f(298\text{ K})$ kJ mol ⁻¹	$\Delta H_f(298\text{ K})$ kcal mol ⁻¹	S(298 K) J K ⁻¹ mol ⁻¹	S(298 K) cal K ⁻¹ mol ⁻¹	Reference ^{a, b, c}
H	217.998±0.006	52.103±.001	114.717±0.002	27.418±.0001	[28]
H ₂	0.00	0.00	130.680±0.003	31.233±0.001	[28]
O(³ P)	249.18±0.10	59.56±0.02	161.059±0.003	38.194±0.001	[28]
O(¹ D)	438.05±0.1	104.70±0.03			[70]
O ₂	0.00	0.00	205.152±0.005	49.033±0.001	[28]
O ₂ (¹ Δ _g)	94.29±0.01	22.54±0.01			[36]
O ₂ (¹ Σ _g ⁺)	156.96±0.01	37.51±0.01			[36]
O ₃	141.8±2	33.9±0.5	239.01	57.12	[33]
OH	37.20±0.38	8.89±0.09	183.74	43.91	[33,87]
HO ₂	13.8±3.3	3.3±0.8	229.1	54.76	[35,58]
H ₂ O	-241.826±0.040	-57.798±0.010	188.835±0.010	45.133±.002	[28]
H ₂ O ₂	-135.88±0.22	-32.48±0.05	234.52	56.05	[33]
N(⁴ S)	472.68±0.40	112.973±0.10	153.301±0.003	36.640±0.001	[28]
N ₂	0.00	0.00	191.609±0.004	45.796±0.001	[28]
NH	357±1	85.3±0.3	181.25±0.04	43.32±0.01	[4]
NH ₂	186±1	44.5±0.3	194.71±0.05	46.54±0.01	[4]
NH ₃	-45.94±0.35	-10.98±0.08	192.77±0.05	46.07±0.01	[28]
NH ₂ OH	-40.2±9.2	-9.6±2.2	236.18	56.45	[5]
NH ₂ NO ₂	-26±10	-6.2±3	268.54	64.18	[33]
NO	91.29±0.17	21.82±0.04	210.76	50.37	[5,22]
N ₂ O	81.6±0.5	19.50±0.12	220.01	52.58	[33]
NO ₂	34.19±0.5	8.17±0.1	240.17	57.40	[33]
NO ₃	73.7±1.4	17.6±0.3	258.4±1.0	61.76±0.24	[1,29]
N ₂ O ₃	86.6±1	20.7±0.3	314.74	75.22	[33]
N ₂ O ₄	11.1±1	2.65±0.25	340.45	81.37	[33]
N ₂ O ₅	13.3±1.5	3.18±0.36	355.7±7	85.01±2	[33]
HNO	107.1±2.5	25.6±0.6			[5]

SPECIES	$\Delta H_f(298\text{ K})$ kJ mol ⁻¹	$\Delta H_f(298\text{ K})$ kcal mol ⁻¹	S(298 K) J K ⁻¹ mol ⁻¹	S(298 K) cal K ⁻¹ mol ⁻¹	Reference ^{a, b, c}
HONO	-78.45±0.8	-18.75±0.2	254.07	60.72	[33]
HONO ₂	-133.9±0.6	-32.0±0.1	266.88	63.78	[33]
HO ₂ NO	-23.8	-5.7	274	65.6	[61], calc.
HO ₂ NO ₂	-53.1±2.5	-12.7±0.6	294±3	70.3±0.7	[84]
C	716.68±0.45	171.29±0.11	158.100±0.001	37.787±0.001	[28]
CH	597.37±1.3	142.77±0.3	183.04	43.75	[33]
CH ₂ (³ B ₁)	390.4±0.8	93.31±0.2	194.90	46.58	[88]
CH ₂ (¹ A ₁)	428.0±0.8	102.3±0.2			[39]
CH ₃	146.65±0.29	35.05±0.07	193.96	46.36	[33,88]
CH ₄	-74.48±0.41	-17.80±0.10	186.38	44.55	[31,82]
CN	440±5	105±1	202.64	48.43	[33]
HCN	132±4	31.5±1	201.82	48.24	[33]
C ₂ N ₂	309.1±0.8	73.9±0.2	242.20	57.89	[33]
CH ₂ NH ₂	149±8	35.6±2			[62], corr.
CH ₃ NH ₂	-23.4±1.0	-5.6±0.3	242.89	58.05	[31,79]
CH ₂ NO	157±4	37.5±1			[96], calc.
NH ₂ CO	-15.1±4	-3.6±1			[96], calc.
NCO	151±14	36±3	232.38	55.54	[75], corr., [33]
HNCO	-104±12	-24.8±2.8	237.97±0.8	56.9±0.2	[97], corr., [102]
CO	-110.53±0.17	-26.42±0.04	197.660±0.004	47.242±0.001	[28]
CO ₂	-393.51±0.13	-94.05±0.03	213.785±0.010	51.096±0.002	[28]
HCO	44.15±0.43	10.55±0.10	224.34	53.62	[8], corr., [33]
CH ₂ O	-108.7±0.05	-25.98±0.01	218.76	52.28	[33]
HCOO	127	30	244.7	58.5	[106], calc.
C(O)OH	-193	-45	251.6	60.1	[106]
HC(O)OH	-378.8±0.5	-90.54±0.1	248.87	59.48	[33,106]
CH ₃ O	17.15±3.8	4.1±0.9	232.86	55.655	[11,33]
CH ₃ O ₂	9.0±5.1	2.15±1.2			[46]
CH ₂ OH	-11.5±1.3	-2.75±0.31	244.170±0.018	58.358±0.004	[41]
CH ₃ OH	-201.0±0.6	-48.04±0.14	239.865	57.329	[33]
CH ₃ OOH	-139.0±8.1	-33.2±1.9			[46]
CH ₂ NO ₂	147.3	35.2	272.48	65.12	[31]
CH ₃ NO ₂	-74.3±0.6	-17.8±0.2	275.2	65.8	[31,79]
CH ₃ ONO	-64.0	-15.3	284.3	67.95	[98]
CH ₃ ONO ₂	-122.2±4.3	-29.2±1.1	301.9	72.15	[79,98]
C ₂ H	565.3±2.9	135.1±0.7	209.73	50.13	[11,33]
C ₂ H ₂	227.4±0.8	54.35±0.2	200.93	48.02	[33]
C ₂ H ₂ OH	121±11	28.9±2.6			[32]
C ₂ H ₃	299±5	71.5±1			[99]
C ₂ H ₄	52.4±0.5	12.52±0.12	219.316	52.418	[33]
C ₂ H ₅	120.9±1.7	28.9±0.4	250.52	59.88	[11,33]
C ₂ H ₆	-83.85±0.29	-20.04±0.07	229.162	54.771	[33,82]
CH ₂ CN	252.6±4	60.4±1.0			[52]
CH ₃ CN	74.04±0.37	17.70±0.09	245.12±0.8	58.59±0.2	[2,102]
CH ₂ CO	-49.58±0.88	-11.85±0.21			[88]
CH ₃ CO	-10.0±1.2	-2.4±0.3			[11]
CH ₂ CHO	10.5±9.2	2.5±2.2			[11]
CH ₃ CHO	-166.1±0.5	39.7±0.1	263.95	63.09	[31,79]
CH ₃ CH ₂ O	-15.5±3.3	-3.7±0.8			[11]
(CHO) ₂	-212±0.8	-50.7±0.2			[30]

SPECIES	$\Delta H_f(298\text{ K})$ kJ mol ⁻¹	$\Delta H_f(298\text{ K})$ kcal mol ⁻¹	S(298 K) J K ⁻¹ mol ⁻¹	S(298 K) cal K ⁻¹ mol ⁻¹	Reference ^{a, b, c}
C ₂ H ₅ O	-17.2	-4.1			[62]
C ₂ H ₅ O ₂	-27.4±9.9	-6.6±2.4			[46]
C ₂ H ₅ OOH	-175.4±12.9	-41.9±3.1			[46]
CH ₂ CH ₂ OH	-31±7	-7.5±1.7			[32]
CH ₃ CHOH	-63.7±4	-15.2±1			[62]
C ₂ H ₅ OH	-234.8±0.5	-56.12±0.12	281.622	67.309	[33]
CH ₃ COO	-190	-45	284.9	68.1	[106], calc.
CH ₂ C(O)OH	-243	58	238.4	57.0	[106]
CH ₃ C(O)O	-192.5	-46.0			[63], calc.
CH ₃ C(O)OH	-432.8±0.5	-103.4±0.1	332.67	79.51	[18,79]
CH ₃ C(O)O ₂	-154.4	-36.9			[63], calc.
CH ₃ C(O)O ₂ NO ₂	-240.1	-57.4			[63], calc.
HOCH ₂ COOH	-583±10	-139±3	318.6±5.0	76.1±1.2	[30]
CH ₃ OCH ₂	-13.0±4	-3.1±1			[62], corr.
CH ₃ OCH ₃	-184.1±0.5	-44.0±0.1	267.34	63.90	[31,79]
CH ₂ (OH)CH ₂ OH	-392.2±4.0	93.7±1.0	303.81	72.61	[31,79]
CH ₃ OOCH ₃	-125.5±5.0	-30.0±1.2			[30]
(HOCO) ₂	-731.8±2.0	-174.9±0.5	320.6±5.0	76.6±1.2	[30]
C ₃ H ₅	166.1±4.3	39.7±1.0	248±15	59.3±3.6	[94]
C ₃ H ₆	20.0±0.7	4.78±0.2	266.6	63.72	[17,79]
n-C ₃ H ₇	100±2	24±0.5			[99]
i-C ₃ H ₇	86.6±2.0	20.7±0.5	281±5	67.2±1.2	[95]
i-C ₃ H ₇ O ₂	-65.4±11.3	-15.6±2.7			[46]
C ₃ H ₈	-104.68±0.50	-25.02±0.12	270.20	64.58	[16,82]
C ₂ H ₅ CHO	-185.6±0.8	44.4±0.2	304.51		[31,79]
CH ₃ COCH ₃	-217.1±0.7	51.9±0.2	295.46	70.62	[31,79]
n-C ₄ H ₁₀	-125.65±0.67	-30.03±0.16	309.91	74.07	[31,82]
(CH ₃ COO) ₂	-500±10	-120±3	390.7±6.0	93.4±1.4	[30]
F	79.38±0.30	18.94±0.07	158.751±0.004	37.942±0.001	[28]
F ₂	0.00	0.00	202.791±0.005	48.468±0.001	[28]
HF	-273.30±0.70	-65.32±0.17	173.799±0.003	41.539±0.001	[28]
HOF	-98.3±4.2	-23.5±1.0	226.77±0.21	54.20±0.05	[22]
FO	109±10	26±3	216.40±0.3	51.72±0.07	[21]
FOF	24.5±2	5.86±0.5	247.46±0.4	59.14±0.1	[21]
OFO	380±20	90.8±5	251±1	60.0±0.3	[21], calc.
FOO	25.4±2	6.07±0.5	259.5±0.2	62.02±0.05	[21]
FOOF	19.2±2.0	4.59±0.5	277.2±0.2	66.25±0.05	[21]
FONO	67	16			[6], est
FNO	-65.7	-15.70	248.0	59.27	[98]
FNO ₂	-79	-19.0	277.1	66.24	[98]
FONO ₂	10±2	2.5±0.5	290	70	[22], est.
CF	244.1±10	58.3±2.4	213.03±0.04	50.92±0.01	[22,33]
CHF	143.1±12	34.2±3.0	234.87	56.14	[33,83]
CF ₂	-184±8	-44.0±2	240.83±0.04	57.56±0.01	[22,83]
CF ₃	-465.7±2.1	-111.3±0.5	264.56	63.23	[33,89]
CF ₄	-933.20±0.75	-223.04±0.18	261.454	62.49	[28]
CHF ₃	-692.9±2.1	-165.6±0.5	259.67	62.06	[33,89]
CHF ₂	-239±4	-57.1±1.0	258.50	61.78	[81]
CH ₂ F ₂	-452.7±0.8	-108.2±0.2	246.59	58.94	[85]
CH ₂ F	-32±8	-7.6±2	236.52	56.53	[81]

SPECIES	$\Delta H_f(298\text{ K})$ kJ mol ⁻¹	$\Delta H_f(298\text{ K})$ kcal mol ⁻¹	S(298 K) J K ⁻¹ mol ⁻¹	S(298 K) cal K ⁻¹ mol ⁻¹	Reference ^{a, b, c}
CH ₃ F	-238±8	-56.8±2	222.78	53.246	[85], H est.
FCO	-161.2±8.1	-38.5±2.0			[44]
CHFO	-383±7	-91.6±1.7	246.82	58.99	[91], calc., [33]
CF ₂ O	-607.9±7.1	-145.3±1.7	258.97	61.89	[91], calc., [33]
CF ₃ O	-624±8	-149±2			[91], calc.
CF ₂ O ₂	-427±6	-102±1.5			[48], calc.
CF ₃ O ₂	-612.5±15.4	146±4			[56]
CF ₃ OH	-911±8	-218±2			[91]
CF ₃ OOCF ₃	-1434±11	-343±3			[91]
CF ₃ OF	-724±8	-173±2			[91]
CH ₂ CH ₂ F	59.4±8	-14.2±2	279.7	66.86	[66],[25], calc.
CH ₃ CHF	-70.3±8	-16.8±2	274.0	65.48	[66], [26], calc.
CH ₃ CH ₂ F	-277.4±4.2	-66.3±1	265.1	63.4	[59], est. [33]
CH ₂ FCH ₂ F	-432±25	-103.2±6			[42]
CH ₂ FCHF	235.5	56.28	293.3	70.11	[27]
CH ₂ FCHF ₂	-665±4	-158.9±1			[51], corr.
CHF ₂ CHF ₂	-860±24	-205.6±5.7	320.3	76.6	[64], corr. [31]
CH ₂ CF ₃	-517.1±5	-123.6±1.2	306.8	73.32	[25,104]
CH ₃ CF ₃	-745.6±1.7	-178.2±0.4	287.3	68.67	[23]
CHF ₂ CH ₂	-277	-66.3	297.8	71.17	[25], calc.
CH ₃ CF ₂	-302.5±8.4	-72.3±2	290.3	69.39	[80], [26], S calc
CH ₃ CHF ₂	-500.1±6.3	-119.7±1.5	282.4	67.50	[23]
CHFCF ₃	-697	-166.5	326.2	77.97	[27], H corr.
CH ₂ FCF ₃	-896±8	-214.1±2	316.2	75.58	[23], H est.
CF ₂ CF ₃	-891±5	-213±1.3			[105]
CHF ₂ CF ₃	-1105±5	-264±1.1	333.7	79.76	[23]
C ₂ F ₆	-1344.3±3.4	-321.3±0.8	331.8	79.30	[23,89]
Cl	121.301±0.008	28.992±0.002	165.190±0.004	39.481±0.001	[28]
Cl ₂	0.00	0.00	223.081±0.010	53.318±0.002	[28]
HCl	-92.31±0.10	-22.06±0.02	186.902±0.005	44.671±0.001	[28]
ClO	101.63±0.1	24.29±0.03	225.07±0.5	53.79±0.12	[22]
ClOO	98.0±4	23.4±1	269.32±0.5	64.37±0.1	[22]
OCIO	94.6±1.2	22.6±0.3	256.84±0.1	61.39±0.03	[22,72]
ClO ₃	194±12	46±3	270.75±0.5	64.71±0.1	[22]
ClClO	90±30	22±7	278.8±2.0	66.6±0.5	[22]
ClOCl	81.3±1.8	19.4±0.4			[34]
ClOOCl	127.6±2.9	30.5±0.7	301.0±5.0	71.9±1.2	[22,72]
ClClO ₂	154.2	36.9	294±2	70.3±0.5	[55], calc., [22]
ClOClO	175.5	41.9	309±2	73.9±0.5	[55], calc., [22]
Cl ₂ O ₃	150±6	35.8±1.5	390±20	94±5	[14]
HOCl	-74.8±1.2	-17.9±0.3	236.50±0.42	56.52±0.10	[22,34]
ClNO	52.7±0.5	12.6±0.1	261.58	62.52	[33]
ClNO ₂	12.5±1.0	3.0±0.3	272.23	65.06	[33]
cis-ClONO	-64.4±6.3	15.4±1.5			[54], calc.
trans-ClONO	75.3±6.3	18.0±1.5			[54], calc.
ClO ₂ NO	102	24.3	316	75.5	[61], calc.
ClONO ₂	22.9±2.0	5.5±0.5	302.38	72.27	[3]
FCl	-55.70±0.31	13.31±0.07	217.94	52.09	[33]
CHCl	326±8	78.0±2.0	234.88	56.85	[33,83]
CCl ₂	230±8	55.0±2.0	265.03	63.34	[33,83]

SPECIES	$\Delta H_f(298\text{ K})$ kJ mol ⁻¹	$\Delta H_f(298\text{ K})$ kcal mol ⁻¹	S(298 K) J K ⁻¹ mol ⁻¹	S(298 K) cal K ⁻¹ mol ⁻¹	Reference ^{a, b, c}
CCl ₃	71.1±2.5	17.0±0.6	303.24	72.47	[37]
CCl ₃ OH	-293±20	-70.0±5			[90], calc.
CCl ₃ O	-43.5±20	-10.4±5			[90], calc
CCl ₃ O ₂	-20.9±8.9	-5.0±2.1			[46]
CCl ₄	-95.6±2.5	-22.8±0.6	309.90	74.069	[38,85][60]
CHCl ₃	-102.9±2.5	-24.6±0.6	295.51	70.63	[60,85]
CHCl ₂	89.0±3.0	21.3±0.7	280±7	66.9±2	[92]
CHCl ₂ O ₂	-17±7	-4±2			[92]
CH ₂ Cl	117.3±3.1	28.0±0.7	271±7	64.5±2	[92]
CH ₂ ClO ₂	-4±11	-1±3			[92]
CH ₂ Cl ₂	-95.1±2.5	-22.8±0.6	270.31	64.606	[60,85]
CH ₃ Cl	-81.9±0.6	-19.6±0.2	227.15	54.290	[60,85]
CICO	-24.9±4.2	-5.9±1.0	266.0	63.6	[22,57]
CHClO	-164±20	-38±5	259.07	61.92	[33], H est,
CCl ₂ O	-220.9	-52.8	283.8	67.82	[98]
CHFCI	-61±10	-14.5±2.4			[100]
CH ₂ FCI	-264±8	-63.2±2	264.3	63.17	[24,100], H est.
CFCI	31±13	7.4±3.2	259.032	61.91	[33,83]
CFCI ₂	-89.1±10.0	-21.3±2.4			[100]
CFCI ₃	-285.3	-68.2	309.9	74.06	[24], corr.
CF ₂ Cl ₂	-494.1	-118.1	300.7	71.87	[24], corr.
CF ₃ Cl	-709.2±2.9	-169.5±0.7	285.2	68.16	[24,89]
CHFCI ₂	-285±9	-68.1±2.1	293.0	70.04	[24], H est.
CHF ₂ Cl	-484.8	-115.6	280.8	67.11	[24], H est.
CF ₂ Cl	-279±8	-66.7±2			[68]
CFCIO	-429±20	-103±5	276.70	66.13	[33]
CH ₂ CICOOH	-427.6±1.0	-102.2±0.2	325.9±5.0	77.9±1.2	[30]
C ₂ H ₃ Cl	22±3	5.3±0.7			[60]
CH ₃ CHFCI	-313.4±2.6	-74.9±0.6			[47]
CH ₂ CF ₂ Cl	-318	-75.9	322.08	76.98	[77]
CH ₃ CF ₂ Cl	-536.2±5.2	-128.2±1.2	307.1	73.41	[47,77]
C ₂ Cl ₄	-18.8±4	-4.5±1	341.03	81.51	[33,38]
1,1-C ₂ H ₂ Cl ₂	2.4±2.0	0.6±0.5			[60]
Z-1,2-C ₂ H ₂ Cl ₂	-3±2	-0.7±0.5			[60]
E-1,2-C ₂ H ₂ Cl ₂	-0.5±2.0	-0.1±0.5			[60]
C ₂ HCl ₃	-19.1±3.0	-6±0.7	325.20	77.72	[31,78]
CH ₂ CCl ₃	71.5±8	17.1±2			[86]
1,1,1-C ₂ H ₃ Cl ₃	-144.6±2.0	-34.6±0.5	320.03	76.488	[15,47,60]
1,1,2-C ₂ H ₃ Cl ₃	-148.0±4.0	-35.4±0.9			[60]
1,1,1,2-C ₂ H ₂ Cl ₄	-152.3±2.4	-36.4±0.6			[60]
1,1,2,2-C ₂ H ₂ Cl ₄	-156.7±3.5	-37.5±0.8			[60]
C ₂ HCl ₅	-155.9±4.3	-37.3±1.0			[60]
CH ₃ CCl ₂	42.5±1.7	10.2±0.4	288±5	68.8±1.1	[92]
CH ₃ CCl ₂ O ₂	-69.7±4	-16.7±1			[45], corr.
CH ₃ CHCl ₂	-130.6±3.0	-31.2±0.7	305.05	72.908	[15,47]
CH ₂ CH ₂ Cl	93.0±2.4	22.2±0.6	271±7	64.8±2	[93]
CH ₃ CHCl	76.5±1.6	18.2±0.4	279±6	66.7±1.4	[92]
CH ₃ CH ₂ Cl	-112.1±0.7	-26.8±0.2	275.78	65.913	[15,60]
C ₂ Cl ₆	-142±4	-34.0±1	398.62	95.27	[33,38]
Br	111.870±12	26.74±0.03	175.018±0.004	41.830±0.001	[28]

SPECIES	$\Delta H_f(298\text{ K})$ kJ mol ⁻¹	$\Delta H_f(298\text{ K})$ kcal mol ⁻¹	S(298 K) J K ⁻¹ mol ⁻¹	S(298 K) cal K ⁻¹ mol ⁻¹	Reference ^{a, b, c}
Br ₂ (g)	30.91±0.11	7.39±0.03	245.468±0.005	58.668±0.001	[28]
HBr	-36.29±0.16	-8.67±0.04	198.700±0.004	47.490±0.001	[28]
Br ₂ O	106.2±2.5	25.4±0.6			[34]
HOBr	-60.5±1.1	-14.5±0.3			[34]
BrO	126.2±1.7	30.2±0.4	232.97±0.1	55.681±0.023	[19,103]
OBrO	163.9±4.4	39.2±1.1	271±2	64.8±0.5	[19,43], est.
BrOO	108±40	26±10	289±3	69.1±0.7	[19]
BrO ₃	221±50	53±12	285±2	68.1±0.5	[19], est.
BrOBr	107.6±3.5	25.7±0.8	290.8±2	69.50±0.48	[19]
BrBrO	168±20	40±5	313±2	74.8±0.5	[19], est.
BrNO	82.17±0.8	19.64±0.2	273.66±0.8	65.41±0.2	[102]
Z-BrONO	71.9	17.19			[53], calc.
E-BrONO	88.3	21.1			[53], calc.
BrNO ₂	45.2	10.8			[53], calc.
BrONO ₂	42.3±6.3	10.1±1.5			[76]
BrF	-58.9±1.0	-14.08±0.3	228.985	54.729	[33]
BrCl	14.79±0.16	3.53±0.04	240.046	57.372	[33]
CH ₂ Br	169±4	40.4±1.0			[100]
CHBr ₃	23.8±4.5	5.7±1.1	330.67	79.03	[13]calc.,[33]
CHBr ₂	188.9	45.0±2.2			[100]
CBr ₃	235±25	56±6	334.57	80.0	[33]
CH ₂ Br ₂	-11.1±5.0	-2.7±1.2	294	70.23	[13], calc.
CH ₃ Br	-37.7±1.5	-9.02±0.36	245.85±0.25	58.76±0.06	[49]
CH ₂ CH ₂ Br	135.6±6.7	32.4±1.6			[10]
CH ₃ CHBr	127±4	30.4±1			[67] corr.
CH ₃ CH ₂ Br	-61.5±1.0	-14.7±0.3	287.3±0.4	68.66±0.09	[47,50]
CH ₃ CBr ₂	140.2±5.4	33.5±1.3			[69]
CH ₃ CBr ₂ H	26.7±1.9	6.4±0.5			[47]
CF ₃ Br	-641.4±2.3	-153.3±0.5			[89]
CBr ₄	83.9±3.4	20.0±0.8	358.06	85.6	[13,33]
CH ₂ BrCOOH	-383.5±3.1	-91.7±0.7	337.0±5.0	80.5±1.2	[30]
I	106.76±0.04	25.52±0.01	180.787±0.004	43.209±0.001	[28]
I ₂	62.42±0.08	14.92±0.02	260.687±0.005	62.306±0.001	[28]
HI	26.50±0.10	6.33±0.03	206.590±0.004	49.376±0.001	[28]
HOI	-69.6±5.4	-16.6±1.3	255.0±0.1	60.95±0.03	[12,34]
IO	115.9±5.0	27.7±1.2	239.6±0.1	57.27±0.03	[9,34]
OIO	77±15	18±4	279.9	66.9	[65], calc.
IOO	96.6±15	23±4	308.4	73.7	[65], calc.
IO ₃	242±50	58±12	293±4	70.0±1.0	[20], est.
IOI	92.4±15	22.1±4	306.5	73.3	[65]
IIO	134.1±15	32.1±4	317.8	76.0	[65]
IOOI	156.8±15	37.5±4	337.0	80.5	[65], calc.
IIOO	103.0±15	24.6±4	339.9	81.2	[65], calc.
IOIO	124.2±15	29.7±4	349.7	83.6	[65], calc.
OIOO	224.0±15	53.5±4	356.3	85.2	[65], calc.
INO	121±4	29.0±1	282.8±4	67.6±1	[101]

SPECIES	$\Delta H_f(298\text{ K})$ kJ mol ⁻¹	$\Delta H_f(298\text{ K})$ kcal mol ⁻¹	S(298 K) J K ⁻¹ mol ⁻¹	S(298 K) cal K ⁻¹ mol ⁻¹	Reference ^{a, b, c}
INO ₂	60.2±4	14.4±1	294±6	70.3±1.5	[101]
ICI	17.506±0.105	4.184±0.025	427.567	102.191	[22]
IBr	40.88±0.08	9.77±0.02	258.95	61.89	[22]
CH ₃ I	13.76±0.12	3.29±0.03	253.70±0.25	60.635±0.06	[49]
CH ₂ I ₂	118.4±0.1	28.30±0.03	309.41±1.34	73.95±0.32	[49]
CF ₃ I	-586.2±2.1	-140.1±0.5	307.78	73.56	[33,89]
CH ₃ CH ₂ I	-7.5±0.9	-1.79±0.2	295.52±0.42	70.63±0.10	[47,50]
S	277.17±0.15	66.25±0.04	167.829±0.006	40.112±0.002	[28]
S ₂	128.6±0.3	30.74±0.07	228.167±0.010	54.533±0.003	[28]
HS	142.80±2.85	34.13±0.68	195.55	46.74	[74], corr., [33]
H ₂ S	-20.6±0.5	-4.92±0.12	205.81±0.05	49.19±0.01	[28]
SO	4.78±0.25	1.14±0.06	221.94	53.04	[33]
SO ₂	-296.81±0.20	-70.94±0.05	248.223±0.050	59.327±0.012	[28]
SO ₃	-395.9±0.7	-94.62±0.17	256.541	61.315	[33]
HSO	-6.1±2.9	-1.5±0.7			[7]
H ₂ SO ₄	-733±2	-175.2±0.5	299.282	71.530	[33]
CS	279.775±0.75	66.87±0.18	210.55	50.32	[33]
CS ₂	116.7±1.0	27.9±0.2	237.882	56.855	[33]
CS ₂ OH	110.5±4.6	26.4±1.1	321±20	77±5	[71]
CH ₃ S	125.0±1.8	29.87±0.44			[73], corr.
CH ₃ SH	-22.9±0.7	-5.47±0.17	255.14	60.98	[31,79]
CH ₂ SCH ₃	136.8±5.9	32.7±1.4			[40]
CH ₃ SCH ₃	-37.4±0.6	-8.94±0.2	285.96	68.35	[31,79]
CH ₃ SSCH ₃	-24.7±1.0	-5.9±0.3	336.80	80.50	[31,79]
OCS	-141.7±2	-33.9±0.5	231.644	55.36	[33]

Notes:

- Error limits are estimates from the original references.
- If two references are given for a substance, the first refers to the enthalpy value while the second to the entropy.
- The terms “calc” and “est” indicate that the value is calculated or estimated. The term “corr” indicates that an enthalpy value has been adjusted to reflect the value chosen in this table for a reference substance.

References

1. Abramowitz, S. and M. W. Chase, 1991, *Pure App. Chem.*, **63**, 1449-1454.
2. An, X. W. and M. Mansson, 1983, *J. Chem. Thermo.*, **15**, 287-293.
3. Anderson, L. C. and D. W. Fahey, 1990, *J. Phys. Chem.*, **94**, 644-652.
4. Anderson, W. R., 1989, *J. Phys. Chem.*, **93**, 530-536.
5. Anderson, W. R., 1999, *Comb. Flame*, **117**, 394-403.
6. Atkinson, R., D. L. Baulch, R. A. Cox, R. F. Hampson, J. A. Kerr, M. J. Rossi and J. Troe, 1997, *J. Phys. Chem. Ref. Data*, **26**, 521-1011.
7. Balucani, N., P. Casavecchia, D. Stranges and G. G. Volpi, 1993, *Chem. Phys. Lett.*, **211**, 469-472.
8. Becerra, R., I. W. Carpenter and R. Walsh, 1997, *J. Phys. Chem.*, **101**, 4185-4190.
9. Bedjanian, Y., G. Le Bras and G. Poulet, 1997, *J. Phys. Chem. A*, **101**, 4088-4096.
10. Bedjanian, Y., G. Poulet and G. Le Bras, 1999, *J. Phys. Chem. A*, **103**, 4026-4033.
11. Berkowitz, J., G. B. Ellison and D. Gutman, 1994, *J. Phys. Chem.*, **98**, 2744-2765.
12. Berry, R., J. Yuan, A. Misra and P. Marshall, 1998, *J. Phys. Chem. A*, **102**, 5182-5188.
13. Bickerton, J., M. E. M. da Piedade and G. Pilcher, 1984, *J. Chem. Thermo.*, **16**, 661-668.
14. Burkholder, J. B., R. K. Talukdar, A. R. Ravishankara and S. Solomon, 1993, *J. Geophys. Res.*, **98**, 22937-22948.
15. Chao, J., A. S. Rodgers, R. C. Wilhoit and B. J. Zvolinski, 1974, *J. Phys. Chem. Ref. Data*, **3**, 141-162.
16. Chao, J., R. C. Wilhoit and B. J. Zvolinski, 1973, *J. Phys. Chem. Ref. Data*, **2**, 427-437.
17. Chao, J. and B. J. Zvolinski, 1975, *J. Phys. Chem. Ref. Data*, **4**, 251-261.
18. Chao, J. and B. J. Zvolinski, 1978, *J. Phys. Chem. Ref. Data*, **7**, 363-377.
19. Chase, M. W., 1996, *J. Phys. Chem. Ref. Data*, **25**, 1069-1111.
20. Chase, M. W., 1996, *J. Phys. Chem. Ref. Data*, **25**, 1297-1340.
21. Chase, M. W., 1996, *J. Phys. Chem. Ref. Data*, **25**, 551-603.
22. Chase, M. W., 1998, *J. Phys. Chem. Ref. Data*, **Monograph 9**.
23. Chen, S. S., A. S. Rodgers, J. Chao, R. C. Wilhoit and B. J. Zvolinski, 1975, *J. Phys. Chem. Ref. Data*, **4**, 441-456.
24. Chen, S. S., R. C. Wilhoit and B. J. Zvolinski, 1976, *J. Phys. Chem. Ref. Data*, **5**, 571-580.
25. Chen, Y., A. Rauk and E. Tschuikow-Roux, 1990, *J. Chem. Phys.*, **93**, 6620-6629.
26. Chen, Y., A. Rauk and E. Tschuikow-Roux, 1990, *J. Chem. Phys.*, **93**, 1187-1195.
27. Chen, Y., A. Rauk and E. Tschuikow-Roux, 1991, *J. Chem. Phys.*, **94**, 7299-7310.
28. Cox, J. D., D. D. Wagman and V. A. Medvedev *CODATA Key Values for Thermodynamics*; Hemisphere Publishing Corp.: New York, 1989.
29. Davis, H. F., B. Kim, H. S. Johnston and Y. T. Lee, 1993, *J. Phys. Chem.*, **97**, 2172-2180.
30. Dorofeeva, O., V. P. Novikov and D. B. Neumann, 2001, *J. Phys. Chem. Ref. Data*, **30**, 475-513.
31. Frenkel, M., G. J. Kabo, K. N. Marsh, G. N. Roganov and R. C. Wilhoit *Thermodynamics of organic compounds in the gas state*; Thermodynamics Research Center: College Station, TX, 1994; Vol. I.
32. Fulle, D., H. F. Hamann, H. Hippler and C. P. Jansch, 1997, *Ber. Bunsenges. Phys. Chem.*, **101**, 1433-1442.
33. Gurvich, L. V., I. V. Veyts and C. B. Alcock *Thermodynamic Properties of Individual Substances*, Fourth ed.; Hemisphere Publishing Corp.: New York, 1991; Vol. 2.
34. Hassanzadeh, P. and K. K. Irikura, 1997, *J. Phys. Chem. A*, **101**, 1580-1587.
35. Hills, A. J. and C. J. Howard, 1984, *J. Chem. Phys.*, **81**, 4458-4465.
36. *Constants of Diatomic Molecules*; Huber, K. P. and G. Herzberg, Eds.; National Institute of Standards and Technology, 1998.
37. Hudgens, J. W., R. D. Johnson, R. S. Timonen, J. A. Seetula and D. Gutman, 1991, *J. Phys. Chem.*, **95**, 4400-4405.
38. Huybrechts, G., M. Marmon and B. Van Mele, 1996, *Int. J. Chem. Kinet.*, **28**, 27-36.
39. Jacox, M. E. *Vibrational and Electronic Energy Levels of Polyatomic Transient Molecules*; National Institute of Standards and Technology, 1998.
40. Jefferson, A., J. M. Nicovich and P. H. Wine, 1994, *J. Phys. Chem.*, **98**, 7128-7135.

41. Johnson, R. D. and J. W. Hudgens, 1996, *J. Phys. Chem.*, **100**, 19874-19890.
42. Kerr, J. A. and D. M. Timlin, 1971, *Int. J. Chem. Kinet.*, **3**, 427-441.
43. Klemm, R. B., R. P. Thorn, L. J. Stief, T. J. Buckley and R. D. Johnson, 2001, *J. Phys. Chem. A*, **105**, 1638-1642.
44. Knyazev, V. D., A. Bencsura and I. R. Slagle, 1997, *J. Phys. Chem. A*, **101**, 849-852.
45. Knyazev, V. D., A. Bencsura and I. R. Slagle, 1998, *J. Phys. Chem. A*, **102**, 1760-1769.
46. Knyazev, V. D. and I. R. Slagle, 1998, *J. Phys. Chem. A*, **102**, 1770-1778.
47. Kolesov, V. P. and T. S. Papina, 1983, *Russ. Chem. Rev.*, **52**, 425-439.
48. Kraka, E., Z. Konkoli, D. Cremer, J. Fowler and H. F. Schaefer, 1996, *J. Amer. Chem. Soc.*, **118**, 10595-10608.
49. Kudchadker, S. A. and A. P. Kudchadker, 1975, *J. Chem. Phys. Ref. Data*, **4**, 457-470.
50. Kudchadker, S. A. and A. P. Kudchadker, 1979, *J. Phys. Chem. Ref. Data*, **8**, 519-526.
51. Lacher, J. R. and H. A. Skinner, 1968, *J. Chem. Soc. A*, 1034-1038.
52. Lafleur, R. D., B. Szatary and T. Baer, 2000, *J. Phys. Chem. A*, **104**, 1450-1455.
53. Lee, J. H., R. B. Timmons and L. J. Stief, 1976, *J. Chem. Phys.*, **64**, 300-305.
54. Lee, T. J., 1994, *J. Phys. Chem.*, **98**, 111-115.
55. Li, W. K. and C. Y. Ng, 1997, *J. Phys. Chem. A*, **101**, 113-115.
56. Lightfoot, P. D., R. A. Cox, J. N. Crowley, M. Destriau, G. D. Hayman, M. E. Jenkin, G. K. Moortgat and F. Zabel, 1992, *Atmos. Environ.*, **26A**, 1805-1961.
57. Lim, K. P. and J. V. Michael, 1994, *J. Phys. Chem.*, **98**, 211-215.
58. Litorja, M. and B. Ruscic, 1998, *J. Electron. Spec. Rel. Phenom.*, **97**, 131-146.
59. Luo, Y. R. and S. W. Benson, 1997, *J. Phys. Chem. A*, **101**, 3042-3044.
60. Manion, J. A., 2002, *J. Phys. Chem. Ref. Data*, **31**, 123-172.
61. McGrath, M. P. and F. S. Rowland, 1994, *J. Phys. Chem.*, **98**, 1060-1067.
62. McMillen, D. F. and D. M. Golden, 1982, *Ann. Rev. Phys. Chem.*, **33**, 493-532.
63. Miller, C. E., J. I. Lynton, D. M. Keevil and J. S. Francisco, 1999, *J. Phys. Chem. A*, **103**, 11451-11459.
64. Millward, G. E., R. Hartig and E. Tschuikow-Roux, 1971, *J. Phys. Chem.*, **75**, 3195-3201.
65. Misra, A. and P. Marshall, 1998, *J. Phys. Chem. A*, **102**, 9056-9060.
66. Miyokawa, K., S. Ozaki and T. Yano, 1996, *Bull. Chem. Soc. Jpn.*, **69**, 869-873.
67. Miyokawa, K. and E. Tschuikow-Roux, 1990, *J. Phys. Chem.*, **94**, 715-717.
68. Miyokawa, K. and E. Tschuikow-Roux, 1992, *J. Phys. Chem.*, **96**, 7328-7331.
69. Miyokawa, K. and E. Tschuikow-Roux, 1999, *Bull. Chem. Soc. Jpn.*, **72**, 1-5.
70. Moore, C. E. *Atomic Energy Levels*; NSRDS: Washington. DC, 1971; Vol. 1.
71. Murrells, T. P., E. R. Lovejoy and A. R. Ravishankara, 1990, *J. Phys. Chem.*, **94**, 2381-2386.
72. Nickolaisen, S. L., R. R. Friedl and S. P. Sander, 1994, *J. Phys. Chem.*, **98**, 155-169.
73. Nicovich, J. M., K. D. Kreutter, C. A. van Dijk and P. H. Wine, 1992, *J. Phys. Chem.*, **96**, 2518-2528.
74. Nicovich, J. M., K. D. Kreutter, C. A. van Dijk and P. H. Wine, 1992, *J. Phys. Chem.*, **96**, 2518-2528.
75. Okabe, H., 1970, *J. Chem. Phys.*, **53**, 3507-3515.
76. Orlando, J. J. and G. S. Tyndall, 1996, *J. Phys. Chem.*, **100**, 19398-19405.
77. Paddison, S. J., Y. H. Chen and E. Tschuikow-Roux, 1994, *Can. J. Chem.*, **72**, 561-567.
78. Papina, T. S. and V. P. Kolesov, 1985, *Russ. J. Phys. Chem.*, **59**, 1289-1292.
79. Pedley, J. B. *Thermochemical Data and Structures of Organic Compounds*; Thermodynamics Data Center: College Station, TX, 1994.
80. Pickard, J. M. and A. S. Rodgers, 1977, *J. Amer. Chem. Soc.*, **99**, 691-694.
81. Pickard, J. M. and A. S. Rodgers, 1983, *Int. J. Chem. Kinet.*, **15**, 569-577.
82. Pittam, D. A. and G. Pilcher, 1972, *J. Chem. Soc. Farad. Trans 1*, **68**, 2224-2229.
83. Poutsma, J. C., J. A. Paulino and R. R. Squires, 1997, *J. Phys. Chem. A*, **101**, 5327-5336.
84. Regimbal, J. M. and M. Mozurkewich, 1997, *J. Phys. Chem. A*, **101**, 8822-8820.
85. Rodgers, A. S., J. Chao, R. C. Wilhoit and B. J. Zwolinski, 1974, *J. Phys. Chem. Ref. Data*, **3**, 117-140.
86. Rodgers, A. S. and P. Jerus, 1988, *Int. J. Chem. Kinet.*, **20**, 565-575.
87. Ruscic, B., D. Feller, D. A. Dixon, K. A. Peterson, L. B. Harding, R. L. Asher and A. F. Wagner, 2001, *J. Phys. Chem. A*, **105**, 1-4.

88. Ruscic, B., M. Litorja and R. L. Asher, 1999, *J. Phys. Chem. A*, **103**, 8625-8633.
89. Ruscic, B., J. V. Michael, P. C. Redfern, L. A. Curtiss and K. Raghavachri, 1998, *J. Phys. Chem. A*, **102**, 10889-10899.
90. Schneider, W. F., B. I. Nance and T. J. Wallington, 1995, *J. Amer. Chem. Soc.*, **117**, 478-485.
91. Schneider, W. F. and T. J. Wallington, 1994, *J. Phys. Chem.*, **98**, 7448-7451.
92. Seetula, J. A., 1996, *J. Chem. Soc. Faraday Trans.*, **92**, 3069-3078.
93. Seetula, J. A., 1998, *J. Chem. Soc. Faraday Trans.*, **94**, 891-898.
94. Seetula, J. A., 1999, *Phys. Chem. Chem. Phys.*, **1**, 4727-4731.
95. Seetula, J. A. and I. R. Slagel, 1997, *J. Chem. Soc. Faraday Trans.*, **93**, 1709-1719.
96. Shapley, W. A. and G. B. Bacskay, 1999, *J. Phys. Chem. A*, **103**, 4505-4513.
97. Spiglanin, T. A., R. A. Pery and D. W. Chandler, 1986, *J. Phys. Chem.*, **90**, 6184-6189.
98. Stull, D. R., E. F. Westrum and G. C. Sinke *The Chemical Thermodynamics of Organic Compounds*; John Wiley & Sons: New York, 1969.
99. Tsang, W. Heats of formation of organic free radicals by kinetic methods. In *Energetics of Free Radicals*; Simoes, J. A. M., Greenberg, A., Liebman, J. F., Eds.; Blackie Academic & Professional: London, 1996; pp 22-58.
100. Tschuikow-Roux, E. and S. Paddison, 1987, *Int. J. Chem. Kinet.*, **19**, 15-24.
101. van den Bergh, H. and J. Troe, 1976, *J. Chem. Phys.*, **64**, 736-742.
102. Wagman, D. D., W. H. Evans, V. B. Parker, R. H. Schumm, I. Halow, S. M. Bailey, K. L. Churney and R. L. Nutall, 1982, *J. Phys. Chem. Ref. Data*, **11**, 392 pp.
103. Wilmouth, D. M., T. F. Hanisco, N. M. Donahue and J. G. Anderson, 1999, *J. Phys. Chem A*, **103**, 8935-8945.
104. Wu, E. C. and A. S. Rodgers, 1974, *J. Phys. Chem.*, **78**, 2315-2317.
105. Wu, E. C. and A. S. Rodgers, 1976, *J. Amer. Chem. Soc.*, **98**, 6112-6115.
106. Yu, D., A. Rauk and D. A. Armstrong, 1994, *J. Chem. Soc. Perkin Trans 2*, 2207-2215.