APPENDIX A. THERMODYNAMIC PARAMETERS

Table of Contents

Tables

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	ΔH_f(298 K) kJ mol^{-1}	ΔH_f(298 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±.0.001	[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]
$O_2(^1\Delta_g)$	94.29±0.01	22.54±0.01			[36]
$O_2(^1\Sigma_g^+)$	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_2O	–241.826±0.040	–57.798±0.010	188.835±0.010	45.133±.002	[28]
H_2O_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_2OH	–40.2±9.2	–9.6±2.2	236.18	56.45	[5]
NH_2NO_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_2O	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_2O_3	86.6±1	20.7±0.3	314.74	75.22	[33]
N_2O_4	11.1±1	2.65±0.25	340.45	81.37	[33]
N_2O_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	ΔH_f(298 K) kJ mol^{-1}	ΔH_f(298 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_2NO	–23.8	–5.7	274	65.6	[61], calc.
HO_2NO_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]
$CH_2(^3B_1)$	390.4±0.8	93.31±0.2	194.90	46.58	[88]
$CH_2(^1A_1)$	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_2N_2	309.1±0.8	73.9±0.2	242.20	57.89	[33]
CH_2NH_2	149±8	35.6±2			[62], corr.
CH_3NH_2	–23.4±1.0	–5.6±0.3	242.89	58.05	[31,79]
CH_2NO	157±4	37.5±1			[96], calc.
NH_2CO	–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_2O	–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_3O	17.15±3.8	4.1±0.9	232.86	55.655	[11,33]
CH_3O_2	9.0±5.1	2.15±1.2			[46]
CH_2OH	–11.5±1.3	–2.75±0.31	244.170±0.018	58.358±0.004	[41]
CH_3OH	–201.0±0.6	–48.04±0.14	239.865	57.329	[33]
CH_3OOH	–139.0±8.1	–33.2±1.9			[46]
CH_2NO_2	147.3	35.2	272.48	65.12	[31]
CH_3NO_2	–74.3±0.6	–17.8±0.2	275.2	65.8	[31,79]
CH_3ONO	–64.0	–15.3	284.3	67.95	[98]
CH_3ONO_2	–122.2±4.3	–29.2±1.1	301.9	72.15	[79,98]
C_2H	565.3±2.9	135.1±0.7	209.73	50.13	[11,33]
C_2H_2	227.4±0.8	54.35±0.2	200.93	48.02	[33]
C_2H_2OH	121±11	28.9±2.6			[32]
C_2H_3	299±5	71.5±.1			[99]
C_2H_4	52.4±0.5	12.52±0.12	219.316	52.418	[33]
C_2H_5	120.9±1.7	28.9±0.4	250.52	59.88	[11,33]
C_2H_6	–83.85±0.29	–20.04±0.07	229.162	54.771	[33,82]
CH_2CN	252.6±4	60.4±1.0			[52]
CH_3CN	74.04±0.37	17.70±0.09	245.12±0.8	58.59±0.2	[2,102]
CH_2CO	–49.58±0.88	–11.85±0.21			[88]
CH_3CO	–10.0±1.2	–2.4±0.3			[11]
CH_2CHO	10.5±9.2	2.5±2.2			[11]
CH_3CHO	–166.1±0.5	39.7±0.1	263.95	63.09	[31,79]
CH_3CH_2O	–15.5±3.3	–3.7±0.8			[11]
$(CHO)_2$	–212±0.8	–50.7±0.2			[30]

SPECIES	ΔH_f(298 K) kJ mol^{-1}	ΔH_f(298 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_2H_5O	–17.2	–4.1			[62]
$C_2H_5O_2$	–27.4±9.9	–6.6±2.4			[46]
C_2H_5OOH	–175.4±12.9	–41.9±3.1			[46]
CH_2CH_2OH	–31±7	–7.5±1.7			[32]
CH_3CHOH	–63.7±4	–15.2±1			[62]
C_2H_5OH	–234.8±0.5	–56.12±0.12	281.622	67.309	[33]
CH_3COO	–190	–45	284.9	68.1	[106], calc.
$CH_2C(O)OH$	–243	58	238.4	57.0	[106]
$CH_3C(O)O$	–192.5	–46.0			[63], calc.
$CH_3C(O)OH$	–432.8±0.5	–103.4±0.1	332.67	79.51	[18,79]
$CH_3C(O)O_2$	–154.4	–36.9			[63], calc.
$CH_3C(O)O_2NO_2$	–240.1	–57.4			[63], calc.
$HOCH_2COOH$	–583±10	–139±3	318.6±5.0	76.1±1.2	[30]
CH_3OCH_2	–13.0±4	–3.1±1			[62], corr.
CH_3OCH_3	–184.1±0.5	–44.0±0.1	267.34	63.90	[31,79]
$CH_2(OH)CH_2OH$	–392.2±4.0	93.7±1.0	303.81	72.61	[31,79]
CH_3OOCH_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_3H_5	166.1±4.3	39.7±1.0	248±15	59.3±3.6	[94]
C_3H_6	20.0±0.7	4.78±0.2	266.6	63.72	[17,79]
n–C_3H_7	100±2	24±0.5			[99]
i–C_3H_7	86.6±2.0	20.7±0.5	281±5	67.2±1.2	[95]
i–$C_3H_7O_2$	–65.4±11.3	–15.6±2.7			[46]
C_3H_8	–104.68±0.50	–25.02±0.12	270.20	64.58	[16,82]
C_2H_5CHO	–185.6±0.8	44.4±0.2	304.51		[31,79]
CH_3COCH_3	–217.1±0.7	51.9±0.2	295.46	70.62	[31,79]
n-C_4H_{10}	-125.65±0.67	-30.03±0.16	309.91	74.07	[31,82]
$(CH_3COO)_2$	–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_2F_2	–452.7±0.8	–108.2±0.2	246.59	58.94	[85]
CH_2F	–32±8	–7.6±2	236.52	56.53	[81]

SPECIES	ΔH_f(298 K) kJ mol^{-1}	ΔH_f(298 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_3F	–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_2O	–607.9±7.1	–145.3±1.7	258.97	61.89	[91],calc., [33]
CF_3O	–624±8	–149±2			[91], calc.
CF_2O_2	–427±6	–102±1.5			[48], calc.
CF_3O_2	-612.5±15.4	146±4			[56]
CF_3OH	–911±8	–218±2			[91]
CF_3OOCF_3	–1434±11	–343±3			[91]
CF_3OF	–724±8	–173±2			[91]
CH_2CH_2F	59.4±8	–14.2±2	279.7	66.86	[66],[25], calc.
CH_3CHF	–70.3±8	–16.8±2	274.0	65.48	[66], [26], calc.
CH_3CH_2F	–277.4±4.2	–66.3±1	265.1	63.4	[59], est. [33]
CH_2FCH_2F	–432±25	–103.2±6			[42]
CH_2FCHF	235.5	56.28	293.3	70.11	[27]
CH_2FCHF_2	–665±4	–158.9±1			[51], corr.
CHF_2CHF_2	–860±24	–205.6±5.7	320.3	76.6	[64], corr. [31]
CH_2CF_3	–517.1±5	–123.6±1.2	306.8	73.32	[25,104]
CH_3CF_3	–745.6±1.7	–178.2±0.4	287.3	68.67	[23]
CHF_2CH_2	–277	–66.3	297.8	71.17	[25], calc.
CH_3CF_2	–302.5±8.4	–72.3±2	290.3	69.39	[80], [26], S calc
CH_3CHF_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_2FCF_3	–896±8	–214.1±2	316.2	75.58	[23], H est.
CF_2CF_3	–891±5	–213±1.3			[105]
CHF_2CF_3	–1105±5	–264±1.1	333.7	79.76	[23]
C_2F_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	101.63v0.1	24.29±0.03	225.07±0.5	53.79±0.12	[22]
ClOO	98.0v4	23.4±1	269.32±0.5	64.37±0.1	[22]
OClO	94.6v1.2	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_2O_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_2NO	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	ΔH_f(298 K) kJ mol^{-1}	ΔH_f(298 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_3OH	–293±20	–70.0±5			[90], calc.
CCl_3O	–43.5±20	–10.4±5			[90], calc
CCl_3O_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]
$CHCl_2O_2$	–17±7	–4!2			[92]
CH_2Cl	117.3±3.1	28.0±0.7	271±7	64.5±2	[92]
CH_2ClO_2	–4v11	–1±3			[92]
CH_2Cl_2	–95.1±2.5	–22.8±0.6	270.31	64.606	[60,85]
CH_3Cl	–81.9±0.6	–19.6±0.2	227.15	54.290	[60,85]
ClCO	–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_2O	–220.9	–52.8	283.8	67.82	[98]
CHFCl	–61±10	–14.5±2.4			[100]
CH_2FCl	–264±8	–63.2±2	264.3	63.17	[24,100], H est.
CFCl	31v13	7.4±3.2	259.032	61.91	[33,83]
$CFCl_2$	–89.1±10.0	–21.3±2.4			[100]
$CFCl_3$	–285.3	–68.2	309.9	74.06	[24], corr.
CF_2Cl_2	–494.1	–118.1	300.7	71.87	[24], corr.
CF_3Cl	–709.2±2.9	–169.5±0.7	285.2	68.16	[24,89]
$CHFCl_2$	–285±9	–68.1±2.1	293.0	70.04	[24], H est.
CHF_2Cl	–484.8	–115.6	280.8	67.11	[24], H est.
CF_2Cl	–279±8	–66.7±2			[68]
CFClO	–429±20	–103±5	276.70	66.13	[33]
$CH_2ClCOOH$	–427.6±1.0	–102.2±0.2	325.9±5.0	77.9±1.2	[30]
C_2H_3Cl	22±3	5.3±0.7			[60]
CH_3CHFCl	–313.4±2.6	–74.9±0.6			[47]
CH_2CF_2Cl	–318	–75.9	322.08	76.98	[77]
CH_3CF_2Cl	–536.2±5.2	–128.2±1.2	307.1	73.41	[47,77]
C_2Cl_4	–18.8±4	–4.5±1	341.03	81.51	[33,38]
1,1–$C_2H_2Cl_2$	2.4±2.0	0.6±0.5			[60]
Z–1,2–$C_2H_2Cl_2$	–3±2	–0.7±0.5			[60]
E–1,2–$C_2H_2Cl_2$	–0.5±2.0	–0.1±0.5			[60]
C_2HCl_3	–19.1±3.0	–.6±0.7	325.20	77.72	[31,78]
CH_2CCl_3	71.5±8	17.1±2			[86]
1,1,1–$C_2H_3Cl_3$	–144.6±2.0	–34.6±0.5	320.03	76.488	[15,47,60]
1,1,2–$C_2H_3Cl_3$	–148.0±4.0	–35.4±0.9			[60]
1,1,1,2–$C_2H_2Cl_4$	–152.3±2.4	–36.4±0.6			[60]
1,1,2,2–$C_2H_2Cl_4$	–156.7±3.5	–37.5±0.8			[60]
C_2HCl_5	–155.9±4.3	–37.3±1.0			[60]
CH_3CCl_2	42.5±1.7	10.2±0.4	288±5	68.8±1.1	[92]
$CH_3CCl_2O_2$	–69.7±4	–16.7±1			[45], corr.
CH_3CHCl_2	–130.6±3.0	–31.2±0.7	305.05	72.908	[15,47]
CH_2CH_2Cl	93.0±2.4	22.2±0.6	271±7	64.8±2	[93]
CH_3CHCl	76.5±1.6	18.2±0.4	279±6	66.7±1.4	[92]
CH_3CH_2Cl	–112.1±0.7	–26.8±0.2	275.78	65.913	[15,60]
C_2Cl_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	ΔH_f(298 K) kJ mol^{-1}	ΔH_f(298 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_2O	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_2Br	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_2Br_2	–11.1±5.0	–2.7±1.2	294	70.23	[13], calc.
CH_3Br	–37.7±1.5	–9.02±0.36	245.85±0.25	58.76±0.06	[49]
CH_2CH_2Br	135.6±6.7	32.4±1.6			[10]
CH_3CHBr	127±4	30.4±1			[67] corr.
CH_3CH_2Br	–61.5±1.0	–14.7±0.3	287.3±0.4	68.66±0.09	[47,50]
CH_3CBr_2	140.2±5.4	33.5±1.3			[69]
CH_3CBr_2H	26.7±1.9	6.4±0.5			[47]
CF_3Br	–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]
$CH_2BrCOOH$	–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	24.6v4	339.9	81.2	[65], calc.
IOIO	124.2±15	29.7±4	349.7	83.6	[65], calc.
OIIO	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	ΔH_f(298 K) kJ mol^{-1}	ΔH_f(298 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]
ICl	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_3I	13.76±0.12	3.29±0.03	253.70±0.25	60.635±0.06	[49]
CH_2I_2	118.4±0.1	28.30±0.03	309.41±1.34	73.95±0.32	[49]
CF_3I	–586.2±2.1	–140.1±0.5	307.78	73.56	[33,89]
CH_3CH_2I	–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±.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_2S	–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_2SO_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_2OH	110.5±4.6	26.4±1.1	321±20	77±5	[71]
CH_3S	125.0±1.8	29.87±0.44			[73], corr.
CH_3SH	–22.9±0.7	–5.47±0.17	255.14	60.98	[31,79]
CH_2SCH_3	136.8±5.9	32.7±1.4			[40]
CH_3SCH_3	–37.4±0.6	–8.94±0.2	285.96	68.35	[31,79]
CH_3SSCH_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:

a. Error limits are estimates from the original references.

b. If two references are given for a substance, the first refers to the enthalpy value while the second to the entropy.

c. 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. Zwolinski, 1974, J. Phys. Chem. Ref. Data, **3**, 141-162.
16. Chao, J., R. C. Wilhoit and B. J. Zwolinski, 1973, J. Phys. Chem. Ref. Data, **2**, 427-437.
17. Chao, J. and B. J. Zwolinski, 1975, J. Phys. Chem. Ref. Data, **4**, 251-261.
18. Chao, J. and B. J. Zwolinski, 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. Zwolinski, 1975, J. Phys. Chem. Ref. Data, **4**, 441-456.
24. Chen, S. S., R. C. Wilhoit and B. J. Zwolinski, 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. Jänsch, 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. Franscisco, 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. *Thermochemicsl 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.