

**APPENDIX 1: GAS PHASE ENTHALPY DATA**

SPECIES	$\Delta H_f(298)$ (Kcal/mol)	SPECIES	$\Delta H_f(298)$ (Kcal/mol)	SPECIES	$\Delta H_f(298)$ (Kcal/mol)	SPECIES	$\Delta H_f(298)$ (Kcal/mol)
H	52.1	C <sub>2</sub> H <sub>4</sub>	12.45	CH <sub>2</sub> FCH <sub>2</sub> F	-107±1	CH <sub>3</sub> CH <sub>2</sub> Cl	-26.8
H <sub>2</sub>	0.00	C <sub>2</sub> H <sub>5</sub>	28.4±0.5	CH <sub>2</sub> FCHF <sub>2</sub>	-159±2	CH <sub>2</sub> CH <sub>2</sub> Cl	22±2
O	59.57	C <sub>2</sub> H <sub>6</sub>	-20.0	CHF <sub>2</sub> CHF <sub>2</sub>	-210±1	CH <sub>3</sub> CHCl	17.6±1
O( <sup>1</sup> D)	104.9	CH <sub>2</sub> CN	58.5±3	CH <sub>2</sub> CF <sub>3</sub>	-124±2	Br	26.7
O <sub>2</sub>	0.00	CH <sub>3</sub> CN	18±3	CH <sub>3</sub> CF <sub>3</sub>	-179±2	Br <sub>2</sub>	7.39
O <sub>2</sub> ( <sup>1</sup> Δ)	22.5	CH <sub>2</sub> CO	-11±3	CH <sub>3</sub> CF <sub>2</sub>	-71±2	HBr	-8.67
O <sub>2</sub> ( <sup>1</sup> Σ)	37.5	CH <sub>3</sub> CO	-2.4±0.5	CH <sub>3</sub> CHF <sub>2</sub>	-120±1	HOBr	-14±2
O <sub>3</sub>	34.1	CH <sub>3</sub> CHO	-39.7	CHF <sub>2</sub> CF <sub>3</sub>	-163±2	BrO	30±2
HO	9.3	C <sub>2</sub> H <sub>5</sub> O	-4.1±1	CH <sub>2</sub> FCF <sub>3</sub>	-214±1	BrNO	19.7
HO <sub>2</sub>	2.8±0.5	CH <sub>2</sub> CH <sub>2</sub> OH	-8±2	CF <sub>2</sub> CF <sub>3</sub>	-213±2	BrONO	25±7
H <sub>2</sub> O	-57.81	C <sub>2</sub> H <sub>5</sub> OH	-56.2	CHF <sub>2</sub> CF <sub>3</sub>	-264±2	BrNO <sub>2</sub>	17±2
H <sub>2</sub> O <sub>2</sub>	-32.60	CH <sub>3</sub> CO <sub>2</sub>	-49.6	Cl	28.9	BrONO <sub>2</sub>	≤11
N	113.00	CH <sub>3</sub> COOH	-103.3	Cl <sub>2</sub>	0.00	BrCl	3.5
N <sub>2</sub>	0.00	C <sub>2</sub> H <sub>5</sub> O <sub>2</sub>	-6±2	HCl	-22.06	CH <sub>2</sub> Br	40±2
NH	85.3	CH <sub>3</sub> COO <sub>2</sub>	-41±5	ClO	24.4	CHBr <sub>3</sub>	6±2
NH <sub>2</sub>	45.3±0.3	CH <sub>3</sub> OOCH <sub>3</sub>	-30.0	ClOO	23.3±1	CHBr <sub>2</sub>	45±2
NH <sub>3</sub>	-10.98	C <sub>3</sub> H <sub>5</sub>	39.4±2	ClOO <sub>2</sub>	>16.7	CBr <sub>3</sub>	48±2
NO	21.57	C <sub>3</sub> H <sub>6</sub>	4.8	ClO <sub>3</sub>	52±4	CH <sub>2</sub> Br <sub>2</sub>	-2.6±2
NO <sub>2</sub>	7.9	n-C <sub>3</sub> H <sub>7</sub>	22.6±2	Cl <sub>2</sub> O	19.5±1	CH <sub>3</sub> Br	-8.5
NO <sub>3</sub>	17.6±1	i-C <sub>3</sub> H <sub>7</sub>	19±3	Cl <sub>2</sub> O <sub>2</sub>	31±3	CH <sub>3</sub> CH <sub>2</sub> Br	-14.8
N <sub>2</sub> O	19.61	C <sub>3</sub> H <sub>8</sub>	-24.8	Cl <sub>2</sub> O <sub>3</sub>	37±3	CH <sub>2</sub> CH <sub>2</sub> Br	32±2
N <sub>2</sub> O <sub>3</sub>	19.8	C <sub>2</sub> H <sub>5</sub> CHO	-44.8	HOCl	-18±3	CH <sub>3</sub> CHBr	30±2
N <sub>2</sub> O <sub>4</sub>	2.2	CH <sub>3</sub> COCH <sub>3</sub>	-51.9	CINO	12.4	I	25.52
N <sub>2</sub> O <sub>5</sub>	2.7±1	CH <sub>3</sub> COO <sub>2</sub> NO <sub>2</sub>	-62±5	CINO <sub>2</sub>	3.0	I <sub>2</sub>	14.92
HNO	25.6±1	F	19.0±0.1	CIONO	13	HI	6.3
HONO	-19.0	F <sub>2</sub>	0.00	CIONO <sub>2</sub>	5.5	CH <sub>3</sub> I	3.5
HNO <sub>3</sub>	-32.3	HF	-65.14±0.2	FCI	-12.1	CH <sub>2</sub> I	52±2
HO <sub>2</sub> NO <sub>2</sub>	-12.5±2	HOF	-23.4±1	CCl <sub>2</sub>	57±5	IO	30.5±2
C	170.9	FO	26±3	CCl <sub>3</sub>	17±1	INO	29.0
CH	142.0	F <sub>2</sub> O	5.9±4	CCl <sub>3</sub> O <sub>2</sub>	-2.7±1	INO <sub>2</sub>	14.4
CH <sub>2</sub>	93±1	FO <sub>2</sub>	6±1	CCl <sub>4</sub>	-22.9	S	66.22
CH <sub>3</sub>	35±0.2	F <sub>2</sub> O <sub>2</sub>	5±2	CHCl <sub>3</sub>	-24.6	S <sub>2</sub>	30.72
CH <sub>4</sub>	-17.88	FONO	13±7	CHCl <sub>2</sub>	23±2	HS	34.2±1
CN	104±3	FNO	-16±2	CH <sub>2</sub> Cl	29±2	H <sub>2</sub> S	-4.9
HCN	32.3	FNO <sub>2</sub>	-26±2	CH <sub>2</sub> Cl <sub>2</sub>	-22.8	SO	1.3
CH <sub>3</sub> NH <sub>2</sub>	-5.5	FONO <sub>2</sub>	3.1±2	CH <sub>3</sub> Cl	-19.6	SO <sub>2</sub>	-70.96
NCO	38±3	CF	61±2	CICO	-5±1	SO <sub>3</sub>	-94.6
HNCO	-25±3	CF <sub>2</sub>	-44±2	COCl <sub>2</sub>	-52.6	HSO	-1±2
CO	-26.42	CF <sub>3</sub>	-112±1	CHFCI	-15±2	HSO <sub>3</sub>	-92±2
CO <sub>2</sub>	-94.07	CF <sub>4</sub>	-223.0	CH <sub>2</sub> FCI	-63±2	H <sub>2</sub> SO <sub>4</sub>	-176
HCO	10±1	CHF <sub>3</sub>	-166.8	CFCl	7±6	CS	67±2
CH <sub>2</sub> O	-26.0	CHF <sub>2</sub>	-58±2	CFCl <sub>2</sub>	-22±2	CS <sub>2</sub>	28.0
COOH	-53±2	CH <sub>2</sub> F <sub>2</sub>	-108.2	CFCl <sub>3</sub>	-68.1	CS <sub>2</sub> OH	26.4
HCOOH	-90.5	CH <sub>2</sub> F	-8±2	CF <sub>2</sub> Cl <sub>2</sub>	-117.9	CH <sub>3</sub> S	29.8±1
CH <sub>3</sub> O	4±1	CH <sub>3</sub> F	-56±1	CF <sub>3</sub> Cl	-169.2	CH <sub>3</sub> SOO	18±2
CH <sub>3</sub> O <sub>2</sub>	4±2	FCO	-41±15	CHFCI <sub>2</sub>	-68.1	CH <sub>3</sub> SO <sub>2</sub>	-57
CH <sub>2</sub> OH	-3.6±1	F <sub>2</sub> CO	-145±2	CHF <sub>2</sub> Cl	-115.6	CH <sub>3</sub> SH	-5.5
CH <sub>3</sub> OH	-48.2	CF <sub>3</sub> O	-150±2	CF <sub>2</sub> Cl	-67±3	CH <sub>2</sub> SCH <sub>3</sub>	32.7±1
CH <sub>3</sub> OOH	-31.3	CF <sub>3</sub> O <sub>2</sub>	-148±2	COFCI	-102±2	CH <sub>3</sub> SCH <sub>3</sub>	-8.9
CH <sub>3</sub> ONO	-15.6	CF <sub>3</sub> OH	-218±3	CH <sub>3</sub> CF <sub>2</sub> Cl	-127±2	CH <sub>3</sub> SSCH <sub>3</sub>	-5.8
CH <sub>3</sub> ONO <sub>2</sub>	-28.6	CF <sub>3</sub> OOCF <sub>3</sub>	-343±5	CH <sub>2</sub> CF <sub>2</sub> Cl	-75±2	OCS	-34
CH <sub>3</sub> O <sub>2</sub> NO <sub>2</sub>	-10.6±2	CF <sub>3</sub> OOH	-191±5	C <sub>2</sub> Cl <sub>4</sub>	-3.0		
C <sub>2</sub> H	135±1	CF <sub>3</sub> OF	-173±5	C <sub>2</sub> HCl <sub>3</sub>	-1.9		
C <sub>2</sub> H <sub>2</sub>	54.35	CH <sub>3</sub> CHF	-17±2	CH <sub>2</sub> CCl <sub>3</sub>	17±2		
C <sub>2</sub> H <sub>2</sub> OH	30±3	CH <sub>3</sub> CH <sub>2</sub> F	-63±2	CH <sub>3</sub> CCl <sub>3</sub>	-34.0		
C <sub>2</sub> H <sub>3</sub>	71±1						