Heats of Formation ΔH_f, BDE data

ΔH_f data: Species		H	F	Cl	Br	I	OH	NH2	CH3	CH_3CH_2	$(CH_3)_2CH$	$(CH_3)_3C$	$H_2C{=}CHCH_2$	$PhCH_2$	Ph	
		52.1	**19.0**	**29.0**	**26.7**	**25.5**	**9.3**	**45.5**	**35.1**	**28.4**	**22.0**	**11.0**	**40.9**	**49.5**	**81.0**	ΔH_f(radical)
		34.7	-59.5	-54.4	-50.9	-45.1	-32.8	27.1	33.3	34.3	28.7	15.2	29.8	26.9	55.7	ΔH_f(anion)
H	**52.1**	0.0	-65.3	-22.1	-8.7	6.3	-57.8	-11.0	-17.9	-20.0	-25.0	-32.1	4.9	12.0	19.8	
13.598	365.7	0.0	-65.3	-22.1	-8.7	6.3	-57.8	-11.0	-17.9	-20.0	-25.0	-32.1	4.9	12.0	19.8	
CH_3	**35.1**	-17.9	-57.1	-20.0	-8.2	3.4	-48.0	-5.5	-20.0	-25.0	-32.1	-40.1	-0.2	7.1	12.0	
9.840	262	-17.9	-57.1	-20.0	-8.2	3.4	-48.0	-5.5	-20.0	-25.0	-32.1	-40.1	-0.2	7.1	12.0	
CH_3CH_2	**28.4**	-20.0	*-66.5*	-26.8	-15.2	-1.7	-56.2	-13.0	-25.0	-30.4	-36.7	-44.4	-5.3	1.9	7.1	
8.117	215.6	-20.0	*-66.5*	-26.8	-15.2	-1.7	-56.2	-13.0	-25.0	-30.4	-36.7	-44.4	-5.3	1.9	7.1	
$(CH_3)_2CH$	**22**	-25.0	-75.4	-34.7	-22.9	-9.5	-65.2	-20.0	-32.1	-36.7	-42.5	-49.0	-11.8	-5.2	0.9	
7.370	191.5	-25.0	-75.4	-34.7	-22.9	-9.5	-65.2	-20.0	-32.1	-36.7	-42.5	-49.0	-11.8	-5.2	0.9	
$(CH_3)_3C$	**11**	-32.1	*-86.0*	-43.0	-31.6	-17.2	-74.7	-28.8	-40.1	-44.4	-49.0	-54.0	-20.0	-12.9	-5.4	
6.700	165.5	-32.1	*-86.0*	-43.0	-31.6	-17.2	-74.7	-28.8	-40.1	-44.4	-49.0	-54.0	-20.0	-12.9	-5.4	
$H_2C{=}CHCH_2$	**40.9**	4.9	-38.7	-1.3	11.4	23.8	-29.6	14.2	-0.2	-5.3	-11.8	-20.0	20.4	27.0	32.1	
8.180	229.5	4.9	-38.7	-1.3	11.4	23.8	-29.6	14.2	-0.2	-5.3	-11.8	-20.0	20.4	27.0	32.1	
$PhCH_2$	**49.5**	12.0	-30.2	4.5	20.0	30.4	-22.6	21.0	7.1	1.9	-5.2	-12.9	27.0	32.4	39.4	
7.242	216.5	12.0	-30.2	4.5	20.0	30.4	-22.6	21.0	7.1	1.9	-5.2	-12.9	27.0	32.4	39.4	
Ph	**81**	19.8	-27.8	13.0	24.7	39.4	-23.0	20.8	12.0	7.1	0.9	-5.4	32.1	39.4	43.1	
8.320	272.9	19.8	-27.8	13.0	24.7	39.4	-23.0	20.8	12.0	7.1	0.9	-5.4	32.1	39.4	43.1	

ΔH_f(radical)
IP(radical) ΔH_f(cation)

Italics = values from Ab Initio G3 theory
*Calculated from group equivalents;
**ΔHf (RF) = -57.1, -66.5, -75.4, and –86.0 kcal/mol for R = Me, Et, iPr, t-Bu;*
*(Kormos, B. F.; Liebman, J. F.; Cramer, C. J., J. Phys. Org. Chem. **2004**, 17, 656.)*
*Calculated from G3 ΔH(atomization);
*Calculated from reported hydrogenation E to make propylbenzene

BDE data: Species		H	F	Cl	Br	I	OH	NH2	CH3	CH_3CH_2	$(CH_3)_2CH$	$(CH_3)_3C$	$H_2C{=}CHCH_2$	$PhCH_2$	Ph	
		52.1	**19**	**29**	**26.7**	**25.5**	**9.3**	**45.5**	**35.1**	**28.4**	**22**	**11**	**40.9**	**49.5**	**81.0**	ΔH_f(radical)
		34.7	-59.5	-54.4	-50.9	-45.1	-32.8	27.1	33.3	34.3	28.7	15.2	29.8	26.9	55.7	ΔH_f(anion)
H	**52.1**	104.2	136.4	103.2	87.5	71.3	119.2	108.6	105.1	100.5	99.1	95.2	88.1	89.6	113.3	
	365.7	400.4	371.5	333.4	323.5	314.3	390.7	403.8	416.9	420	419.4	413	390.6	380.6	401.6	
CH_3	**35.1**	105.1	111.2	84.1	70	57.2	92.4	86.1	90.2	88.5	89.2	86.2	76.2	77.5	104.1	
	262	314.6	259.6	227.6	219.3	213.5	277.2	294.6	315.3	321.3	322.8	317.3	292	281.8	305.7	
CH_3CH_2	**28.4**	100.5	*114*	84.2	70.3	55.6	93.9	86.9	88.5	87.2	87.1	83.8	74.6	76	102.3	
	215.6	270.3	*223*	188	179.9	172.2	239	255.7	273.9	280.3	281	275.2	250.7	240.6	264.2	
$(CH_3)_2CH$	**22**	99.1	116.4	85.7	71.6	57	96.5	87.5	89.2	87.1	86.5	82	74.7	76.7	102.1	
	191.5	251.2	207.4	171.8	163.5	155.9	223.9	238.6	256.9	262.5	262.7	255.7	233.1	223.6	246.3	
$(CH_3)_3C$	**11**	95.2	*116*	83	69.3	53.7	95	85.3	86.2	83.8	82	76	71.9	73.4	97.42	
	165.5	232.3	*192*	154.1	146.2	137.6	207.4	221.4	238.9	244.2	243.2	234.7	215.3	205.3	226.6	
$H_2C{=}CHCH_2$	**40.9**	88.1	*98.6*	71.2	56.2	42.6	79.8	72.2	76.2	74.6	74.7	71.9	61.4	63.4	89.83	
	229.5	259.3	*208.7*	176.4	167.2	160.6	226.3	242.4	263	269.1	270	264.7	238.9	229.4	253.1	
$PhCH_2$	**49.5**	89.6	98.7	74	56.2	44.6	81.4	74	77.5	76	76.7	73.4	63.4	66.6	91.1	
	216.5	239.2	187.2	157.6	145.6	141	206.3	222.6	242.7	248.9	250.4	244.6	219.3	211	232.8	
Ph	**81**	113.3	127.8	96.99	83	67.1	113.3	105.7	104.1	102.3	102.1	97.42	89.83	91.1	118.9	
	272.9	287.8	241.2	205.5	197.3	188.4	263.1	279.2	294.2	300.1	300.7	293.5	270.6	260.4	285.5	