

First Principles Prediction of Enthalpies of Formation for Polycyclic Aromatic Hydrocarbons and Derivatives*

Thomas C. Allison[†] and Donald R. Burgess Jr.[‡]

*Chemical Science Division,
Material Measurement Laboratory,
National Institute of Standards and Technology,
100 Bureau Drive, Stop 8320, Gaithersburg, Maryland, 20899-8320, USA*

Supplementary Material

*Official contribution of the National Institute of Standards and Technology; not subject to copyright in the United States.

[†]email: thomas.allison@nist.gov

[‡]email: donald.burgess@nist.gov

Table S1: Values of the enthalpy of formation $\Delta_f H_{298K}^\circ$ (kJ/mol) computed using the G3MP2B3 and G3B3 model chemistries for PAH molecules.

Name	Formula	CASNO	$\Delta_f H_{298K}^\circ$ G3MP2B3	$\Delta_f H_{298K}^\circ$ G3B3
<i>ortho</i>				
benzene	C ₆ H ₆	71-43-2	77.0	85.1
naphthalene	C ₁₀ H ₈	91-20-3	135.1	147.8
anthracene	C ₁₄ H ₁₀	120-12-7	208.4	226.0
phenanthrene	C ₁₄ H ₁₀	85-01-8	185.4	202.6
naphthacene	C ₁₈ H ₁₂	92-24-0	288.1	310.6
<i>peri</i>				
acenaphthylene	C ₁₂ H ₈	208-96-8	244.6	259.1
biphenylene	C ₁₂ H ₈	259-79-0	400.8	416.3
acenaphthene	C ₁₂ H ₁₀	83-32-9	141.3	153.4
fluorene	C ₁₃ H ₁₀	86-73-7	170.5	185.3
pyrene	C ₁₆ H ₁₀	129-00-0	200.9	219.6
<i>monosubstituted alkyl</i>				
toluene	C ₇ H ₈	108-88-3	44.5	52.1
ethylbenzene	C ₈ H ₁₀	100-41-4	22.8	30.3
prop-1-ylbenzene	C ₉ H ₁₂	103-65-1	0.2	7.8
prop-2-ylbenzene	C ₉ H ₁₂	98-82-8	-4.4	2.8
<i>disubstituted alkyl</i>				
1,2-dimethylbenzene	C ₈ H ₁₀	95-47-6	11.4	18.6
1,3-dimethylbenzene	C ₈ H ₁₀	108-38-3	10.0	17.2
1,4-dimethylbenzene	C ₈ H ₁₀	106-42-3	10.4	17.4
1-ethyl-2-methylbenzene	C ₉ H ₁₂	611-14-3	-8.2	-0.9
1-ethyl-3-methylbenzene	C ₉ H ₁₂	620-14-4	-10.4	-3.5
1-ethyl-4-methylbenzene	C ₉ H ₁₂	622-96-8	-8.9	-2.1
<i>di-phenyl</i>				
phenylbenzene	C ₁₂ H ₁₀	92-52-4	163.1	178.1
4-phenyltoluene	C ₁₃ H ₁₂	644-08-6	130.8	145.3
benzylbenzene	C ₁₃ H ₁₂	101-81-5	148.6	164.2
<i>cycloalkane</i>				
benzocyclopropane	C ₇ H ₆	4646-69-9	372.4	380.7
benzocyclobutane	C ₈ H ₈	694-87-1	192.3	200.6
indan	C ₉ H ₁₀	496-11-7	52.0	59.7
<i>alkenyl</i>				
ethenylbenzene	C ₈ H ₈	100-42-5	138.9	149.2

Name	Formula	CASNO	$\Delta_f H_{298K}^\circ$ G3MP2B3	$\Delta_f H_{298K}^\circ$ G3B3
(<i>E</i>)-propen-1-ylbenzene	C ₉ H ₁₀	873-66-5	107.5	117.2
(<i>Z</i>)-propen-1-ylbenzene	C ₉ H ₁₀	766-90-5	114.7	125.1
propen-2-ylbenzene	C ₉ H ₁₀	98-83-9	107.5	117.3
propen-3-ylbenzene	C ₉ H ₁₀	300-57-2	124.8	135.1
<i>monosubstituted alkynyl</i>				
ethynylbenzene	C ₈ H ₆	536-74-3	308.3	317.6
propyn-1-ylbenzene	C ₉ H ₈	673-32-5	267.3	276.4
1-ethynyl-4-methylbenzene	C ₉ H ₈	766-97-2	272.9	281.8
<i>cycloalkene</i>				
benzocyclobutene	C ₈ H ₆	4026-23-7	398.8	410.1
indene	C ₉ H ₈	95-13-6	150.3	161.0
1,2-dihydronaphthalene	C ₁₀ H ₁₀	447-53-0	114.9	125.4
<i>dialkenyl</i>				
1,2-Diethenylbenzene	C ₁₀ H ₁₀	91-14-5	209.0	221.2
1,3-Diethenylbenzene	C ₁₀ H ₁₀	108-57-6	200.9	213.4
1,4-diethenylbenzene	C ₁₀ H ₁₀	105-06-6	200.0	212.6
buta-1,3-dien-2-ylbenzene	C ₁₀ H ₁₀	2288-18-8	204.9	217.1
<i>dialkynyl</i>				
1,4-Diethynylbenzene	C ₁₀ H ₆	935-14-8	540.4	551.4
<i>alkenynyl</i>				
1-ethynyl-2-ethenylbenzene	C ₁₀ H ₈		370.8	382.7
1-ethynyl-3-ethenylbenzene	C ₁₀ H ₈		370.5	382.3
1-ethynyl-4-ethenylbenzene	C ₁₀ H ₈		369.7	381.4
<i>other</i>				
benzyne	C ₆ H ₄	462-80-6	449.8	461.2
m-benzyne	C ₆ H ₄	1828-89-3	514.8	523.8
p-benzyne	C ₆ H ₄	3355-34-8	560.6	573.9
pentalene	C ₈ H ₆	250-25-9	363.2	374.8
azulene	C ₁₀ H ₈	275-51-4	282.1	296.2
heptalene	C ₁₂ H ₁₀	257-24-9	400.5	417.1

Table S2: Prediction (B3LYP, corrected) of enthalpies of formation ($\Delta_f H_{298K}^\circ$, kJ/mol) for PAH molecules for which no experimental values are known.

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
1 <i>H</i> -benz[<i>de</i>]anthracene	C ₁₇ H ₁₂	199-95-1	289.7
1 <i>H</i> -benz[<i>e</i>]indene	C ₁₃ H ₁₀	232-54-2	224.7
1 <i>H</i> -benz[<i>fg</i>]aceanthrylene	C ₁₉ H ₁₂	193-69-1	352.5
1 <i>H</i> -benz[<i>fj</i>]indene	C ₁₃ H ₁₀	268-40-6	220.4
1 <i>H</i> -benzo[<i>a</i>]cyclopent[<i>h</i>]anthracene	C ₂₁ H ₁₄	240-44-8	360.8
1 <i>H</i> -benzo[<i>cd</i>]fluoranthene	C ₁₉ H ₁₂	42126-84-1	340.4
1 <i>H</i> -benzo[<i>ghi</i>]cyclopenta[<i>pqr</i>]perylene	C ₂₃ H ₁₂	64503-02-2	362.5
1 <i>H</i> -cyclopent[<i>a</i>]anthracene	C ₁₇ H ₁₂	227-50-9	305.2
1 <i>H</i> -cyclopent[<i>b</i>]anthracene	C ₁₇ H ₁₂	259-06-3	300.5
1 <i>H</i> -cyclopenta[<i>a</i>]pyrene	C ₁₉ H ₁₂	42315-22-0	304.4
1 <i>H</i> -cyclopenta[<i>e</i>]pyrene	C ₁₉ H ₁₂	109587-09-9	306.8
1 <i>H</i> -cyclopenta[<i>l</i>]phenanthrene	C ₁₇ H ₁₂	235-92-7	290.1
1 <i>H</i> -dibenz[<i>a,k</i>]anthracene	C ₂₁ H ₁₄	194-84-3	379.2
1 <i>H</i> -indeno[6,7,1- <i>mna</i>]anthracene	C ₁₉ H ₁₂	190-12-5	348.2
1,2-dihydrobenzo[<i>j</i>]aceanthrylene	C ₂₀ H ₁₄	479-23-2	289.4
2 <i>H</i> -benzo[<i>cd</i>]pyrene	C ₁₉ H ₁₂	191-32-2	341.6
2 <i>H</i> -cyclopenta[<i>l</i>]phenanthrene	C ₁₇ H ₁₂	235-91-6	329.2
3 <i>H</i> -benz[<i>e</i>]indene	C ₁₃ H ₁₀	232-55-3	224.4
3 <i>H</i> -benzo[<i>cd</i>]pyrene	C ₁₉ H ₁₂	191-35-5	281.6
4 <i>H</i> -benzo[<i>b</i>]cyclopenta[<i>jkl</i>]triphenylene	C ₂₃ H ₁₄	143255-68-9	367.6
4 <i>H</i> -benzo[<i>b</i>]cyclopenta[<i>mno</i>]chrysene	C ₂₃ H ₁₄	87308-55-2	380.5
4 <i>H</i> -benzo[<i>c</i>]cyclopenta[<i>mno</i>]chrysene	C ₂₃ H ₁₄	87308-56-3	391.2
4 <i>H</i> -benzo[<i>def</i>]cyclopenta[<i>mno</i>]chrysene	C ₂₁ H ₁₂	59004-72-7	345.8
4 <i>H</i> -benzo[<i>hi</i>]chrysene	C ₂₁ H ₁₄	216-54-6	333.5
4 <i>H</i> -cyclopenta[<i>def</i>]chrysene	C ₁₉ H ₁₂	202-98-2	304.4
4 <i>H</i> -cyclopenta[<i>def</i>]phenanthrene	C ₁₅ H ₁₀	203-64-5	245.5
4 <i>H</i> -cyclopenta[<i>def</i>]triphenylene	C ₁₉ H ₁₂	23992-32-7	297.2
4 <i>H</i> -dibenz[<i>a,k</i>]anthracene	C ₂₁ H ₁₄	194-85-4	358.2

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
4 <i>H</i> -dibenzo[<i>a,de</i>]naphthacene	C ₂₅ H ₁₆	198-40-3	385.7
4 <i>H</i> -dibenzo[<i>a,de</i>]pentacene	C ₂₉ H ₁₈	198-45-8	469.4
4 <i>H</i> -indeno[7,1,2- <i>ghi</i>]chrysene	C ₂₃ H ₁₄	87308-62-1	391.7
5 <i>H</i> -benz[<i>fg</i>]acenaphthylene	C ₁₅ H ₁₀	194-27-4	320.4
5 <i>H</i> -benzo[<i>b</i>]cyclopenta[<i>def</i>]chrysene	C ₂₃ H ₁₄	87308-54-1	381.0
5 <i>H</i> -benzo[<i>cd</i>]pyrene	C ₁₉ H ₁₂	191-34-4	287.1
5 <i>H</i> -dibenzo[<i>c,mn</i>]phenanthrene	C ₂₁ H ₁₄	192-11-0	353.8
5 <i>H</i> -indeno[2,1- <i>a</i>]chrysene	C ₂₅ H ₁₆		389.1
6 <i>H</i> -benzo[<i>cd</i>]pyrene	C ₁₉ H ₁₂	191-33-3	262.4
6 <i>H</i> -cyclopenta[<i>ghi</i>]picene	C ₂₃ H ₁₄	195-90-4	361.8
6 <i>H</i> -naphtho[1,2,3- <i>cd</i>]pyrene	C ₂₃ H ₁₄	189-73-1	328.1
7 <i>H</i> -benz[5,6]indeno[1,2- <i>a</i>]phenanthrene	C ₂₅ H ₁₆	908070-09-7	385.9
7 <i>H</i> -benz[5,6]indeno[2,1- <i>a</i>]phenanthrene	C ₂₅ H ₁₆		373.7
7 <i>H</i> -benzo[<i>c</i>]fluorene	C ₁₇ H ₁₂	205-12-9	256.1
7 <i>H</i> -benzo[<i>de</i>]pentacene	C ₂₅ H ₁₆	229-15-2	396.2
7 <i>H</i> -benzo[<i>hi</i>]chrysene	C ₂₁ H ₁₄	216-53-5	319.8
7 <i>H</i> -dibenz[<i>a,kl</i>]anthracene	C ₂₁ H ₁₄	194-83-2	344.2
7 <i>H</i> -dibenzo[<i>b,g</i>]fluorene	C ₂₁ H ₁₄	204-89-7	320.8
7 <i>H</i> -dibenzo[<i>c,g</i>]fluorene	C ₂₁ H ₁₄	194-58-1	353.9
7 <i>H</i> -indeno[1,2- <i>a</i>]phenanthrene	C ₂₁ H ₁₄	198-08-3	321.5
7 <i>H</i> -indeno[1,2- <i>a</i>]pyrene	C ₂₃ H ₁₄	87308-64-3	335.7
8 <i>H</i> -benzo[<i>g</i>]cyclopenta[<i>mno</i>]chysene	C ₂₃ H ₁₄	87308-57-4	384.5
8 <i>H</i> -cyclopenta[<i>b</i>]phenanthrene	C ₁₇ H ₁₂	224-03-3	282.6
8 <i>H</i> -dibenzo[<i>b,fg</i>]pyrene	C ₂₃ H ₁₄	189-71-9	327.9
8 <i>H</i> -dibenzo[<i>b,mn</i>]phenanthrene	C ₂₁ H ₁₄	6542-08-1	311.8
8 <i>H</i> -indeno[1,2- <i>a</i>]anthracene	C ₂₁ H ₁₄	198-95-8	336.3
8 <i>H</i> -indeno[2,1- <i>b</i>]phenanthrene	C ₂₁ H ₁₄	241-28-1	306.7
8 <i>H</i> -tribenzo[<i>a,cd,l</i>]pyrene	C ₂₇ H ₁₆	190-61-4	431.2
9,10[1',2']-benzenoanthracene,	C ₂₀ H ₁₄	477-75-8	331.1
9 <i>H</i> -benz[4,5]indeno[2,1- <i>c</i>]phenanthrene	C ₂₅ H ₁₆	192-77-8	413.4
9 <i>H</i> -benz[5,6]indeno[2,1- <i>c</i>]phenanthrene	C ₂₅ H ₁₆	192-84-7	411.0

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
9 <i>H</i> -benzo[<i>a</i>]cyclopent[<i>z</i>]anthracene	C ₂₁ H ₁₄	226-78-8	356.3
9 <i>H</i> -indeno[1,2- <i>e</i>]pyrene	C ₂₃ H ₁₄	87308-65-4	339.4
9 <i>H</i> -indeno[2,1- <i>c</i>]phenanthrene	C ₂₁ H ₁₄	192-87-0	346.5
9 <i>H</i> -naphtho[1,2,3- <i>cd</i>]perylene	C ₂₇ H ₁₆		424.8
10 <i>H</i> -benz[<i>g</i>]indeno[2,1- <i>a</i>]phenanthrene	C ₂₅ H ₁₆		399.3
11 <i>H</i> -benz[<i>bc</i>]aceanthrylene	C ₁₉ H ₁₂	202-94-8	319.9
11 <i>H</i> -benzo[<i>a</i>]fluorene	C ₁₇ H ₁₂	238-84-6	246.5
11 <i>H</i> -benzo[<i>b</i>]fluorene	C ₁₇ H ₁₂	243-17-4	244.8
11 <i>H</i> -cyclopenta[<i>a</i>]triphenylene	C ₂₁ H ₁₄	196-87-2	376.4
11 <i>H</i> -cyclopenta[<i>ghi</i>]perylene	C ₂₁ H ₁₂	83899-23-4	361.3
11 <i>H</i> -indeno[1,2- <i>a</i>]triphenylene	C ₂₅ H ₁₆	188-69-2	417.3
11 <i>H</i> -indeno[2,1,7- <i>cde</i>]pyrene	C ₂₁ H ₁₂	59004-71-6	319.6
11 <i>H</i> -indeno[2,1- <i>a</i>]phenanthrene	C ₂₁ H ₁₄	220-97-3	309.3
11 <i>H</i> -indeno[2,1- <i>a</i>]pyrene	C ₂₃ H ₁₄	196-36-1	327.4
12 <i>H</i> -dibenzo[<i>b,h</i>]fluorene	C ₂₁ H ₁₄	242-47-7	308.9
12 <i>H</i> -indeno[1,2- <i>b</i>]phenanthrene	C ₂₁ H ₁₄	248-83-9	306.7
13 <i>H</i> -benzo[<i>b</i>]cyclopenta[<i>def</i>]triphenylene	C ₂₃ H ₁₄	197-79-5	368.5
13 <i>H</i> -cyclopenta[<i>pqr</i>]picene	C ₂₃ H ₁₄	87308-60-9	373.4
13 <i>H</i> -cyclopenta[<i>rst</i>]pentaphene	C ₂₃ H ₁₄	87308-59-6	390.9
13 <i>H</i> -dibenz[<i>bc,j</i>]aceanthrylene	C ₂₃ H ₁₄	201-42-3	380.9
13 <i>H</i> -dibenz[<i>bc,l</i>]aceanthrylene	C ₂₃ H ₁₄	87308-61-0	391.2
13 <i>H</i> -dibenzo[<i>a,de</i>]naphth[2,3- <i>h</i>]anthracene	C ₂₉ H ₁₈		558.0
13 <i>H</i> -dibenzo[<i>a,g</i>]fluorene	C ₂₁ H ₁₄	207-83-0	324.2
13 <i>H</i> -dibenzo[<i>a,h</i>]fluorene	C ₂₁ H ₁₄	239-85-0	310.3
13 <i>H</i> -dibenzo[<i>a,i</i>]fluorene	C ₂₁ H ₁₄	239-60-1	314.0
13 <i>H</i> -dibenzo[<i>b,mn</i>]phenanthrene	C ₂₁ H ₁₄	198-30-1	336.0
13 <i>H</i> -indeno[1,2- <i>b</i>]anthracene	C ₂₁ H ₁₄	248-93-1	325.2
13 <i>H</i> -indeno[1,2- <i>c</i>]phenanthrene	C ₂₁ H ₁₄	212-54-4	319.6
13 <i>H</i> -indeno[1,2- <i>l</i>]phenanthrene	C ₂₁ H ₁₄	201-65-0	324.0
13 <i>H</i> -indeno[2,1,7- <i>qra</i>]naphthacene	C ₂₃ H ₁₄	87308-63-2	402.9
13 <i>H</i> -indeno[2,1- <i>a</i>]anthracene	C ₂₁ H ₁₄	223-31-4	326.6

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
15 <i>H</i> -benz[4,5]indeno[1,2- <i>l</i>]phenanthrene	C ₂₅ H ₁₆	873972-33-9	392.5
15 <i>H</i> -cyclopenta[<i>a</i>]phenanthrene	C ₁₇ H ₁₂	219-07-8	286.9
17 <i>H</i> -cyclopenta[<i>a</i>]phenanthrene	C ₁₇ H ₁₂	219-08-9	287.5
aceanthrylene	C ₁₆ H ₁₀	202-03-9	339.8
acenaphtho[1,2,3- <i>cde</i>]pyrene	C ₂₄ H ₁₂	75449-91-1	448.2
acenaphtho[1,2- <i>j</i>]fluoranthene	C ₂₆ H ₁₄	193-21-5	491.4
acenaphtho[1,2- <i>k</i>]cyclopenta[<i>cd</i>]fluoranthene	C ₂₈ H ₁₄	30909-04-7	642.4
acenaphtho[1,2- <i>k</i>]fluoranthene	C ₂₆ H ₁₄	207-02-3	476.7
acephenanthrene	C ₁₆ H ₁₀	201-06-9	312.0
anthra[1,2,3,4- <i>rst</i>]pentaphene	C ₃₂ H ₁₈	31541-07-8	578.2
anthra[1,2- <i>a</i>]aceanthrylene	C ₂₈ H ₁₆	203-06-5	540.0
anthra[1,2- <i>a</i>]anthracene	C ₂₆ H ₁₆	195-00-6	448.2
anthra[1,2- <i>a</i>]benz[<i>j</i>]anthracene	C ₃₀ H ₁₈	115747-59-6	505.1
anthra[1,2- <i>a</i>]naphthacene	C ₃₀ H ₁₈	115747-78-9	534.1
anthra[1,9,8- <i>abcd</i>]benzo[<i>hi</i>]coronene	C ₃₆ H ₁₆	128345-78-8	561.9
anthra[2,1,9,8,7- <i>defghi</i>]benzo[<i>op</i>]pentacene	C ₃₂ H ₁₆	120864-24-6	497.0
anthra[2,1,9,8,7- <i>defghi</i>]benzo[<i>st</i>]pentacene	C ₃₂ H ₁₆	120836-08-0	466.1
anthra[2,1,9,8,7- <i>defghi</i>]benzo[<i>uv</i>]pentacene	C ₃₂ H ₁₆	120836-13-7	476.6
anthra[2,1,9,8- <i>defgh</i>]benzo[<i>rst</i>]pentaphene	C ₃₂ H ₁₆	120836-01-3	476.4
anthra[2,1,9,8- <i>defgh</i>]pentaphene	C ₃₀ H ₁₆	120835-77-0	461.5
anthra[2,1,9,8- <i>opqra</i>]naphthacene	C ₂₆ H ₁₄	92586-98-6	405.6
anthra[2,1,9,8- <i>stuva</i>]pentacene	C ₃₀ H ₁₆	120835-88-3	488.5
anthra[2,1,9- <i>qra</i>]naphthacene	C ₂₈ H ₁₆	189-52-6	458.8
anthra[2,1- <i>a</i>]aceanthrylene	C ₂₈ H ₁₆	203-21-4	520.1
anthra[2,1- <i>a</i>]naphthacene	C ₃₀ H ₁₈	214-16-4	512.4
anthra[2,3- <i>a</i>]coronene	C ₃₆ H ₁₈	5869-17-0	531.8
anthra[3,2,1,9,8- <i>rstuva</i>]benzo[<i>ij</i>]pentaphene	C ₃₂ H ₁₆	120836-16-0	499.6
anthra[3,2,1,9- <i>pqra</i>]benzo[<i>cd</i>]perylene	C ₃₂ H ₁₆	120836-18-2	514.9
anthra[7,8,9,1,2,3- <i>rstuvw</i>]hexaphene	C ₃₂ H ₁₆	120836-14-8	494.2
anthra[8,9,1,2- <i>cdefg</i>]benzo[<i>a</i>]naphthacene	C ₃₀ H ₁₆	120835-82-7	471.0
anthra[8,9,1,2- <i>lmnop</i>]benzo[<i>a</i>]naphthacene	C ₃₀ H ₁₆	120835-87-2	489.1

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
anthra[9,1,2- <i>abc</i>]coronene	C ₃₄ H ₁₆	128345-73-3	492.5
anthra[9,1,2- <i>bcd</i>]perylene	C ₃₀ H ₁₆	120864-21-3	471.2
anthra[9,1,2- <i>cde</i>]benzo[<i>rst</i>]pentaphene	C ₃₄ H ₁₈	188-87-4	533.1
as-indacene	C ₁₂ H ₈	210-65-1	448.0
as-indaceno[2,3- <i>a</i>]phenanthrene	C ₂₄ H ₁₄	24976-60-1	586.3
azulene	C ₁₀ H ₈	275-51-4	271.2
benz[4,10]anthra[1,9,8- <i>abcd</i>]coronene	C ₃₆ H ₁₆	117726-83-7	483.0
benz[5,6]indeno[2,1- <i>a</i>]phenalene	C ₂₄ H ₁₄	76727-41-8	437.6
benz[<i>a</i>]aceanthrylene	C ₂₀ H ₁₂	203-33-8	363.5
benz[<i>a</i>]acephenanthrylene	C ₂₀ H ₁₂	192-28-9	394.0
benz[<i>a</i>]indeno[1,2- <i>c</i>]fluorene	C ₂₄ H ₁₄	199-21-3	590.7
benz[<i>a</i>]indeno[2,1- <i>c</i>]naphthalene	C ₂₄ H ₁₄	193-27-1	519.6
benz[<i>a</i>]indeno[5,6- <i>g</i>]fluorene	C ₂₄ H ₁₄	192-89-2	607.9
benz[<i>a</i>]ovalene	C ₃₆ H ₁₆	75449-88-6	474.9
benz[<i>b</i>]indeno[2,1- <i>h</i>]fluorene	C ₂₄ H ₁₄	102634-38-8	507.6
benz[<i>c</i>]indeno[2,1- <i>a</i>]fluorene	C ₂₄ H ₁₄	201-72-9	590.4
benz[<i>def</i>]indeno[1,2,3- <i>hi</i>]chrysene	C ₂₆ H ₁₄	111189-33-4	432.0
benz[<i>def</i>]indeno[1,2,3- <i>qr</i>]chrysene	C ₂₆ H ₁₄	111189-34-5	435.5
benz[<i>de</i>]indeno[2,1- <i>b</i>]anthracene	C ₂₄ H ₁₄	32881-40-6	512.3
benz[<i>d</i>]aceanthrylene	C ₂₀ H ₁₂	19770-52-6	423.9
benz[<i>d</i>]ovalene	C ₃₆ H ₁₆	75449-89-7	486.0
benz[<i>e</i>]aceanthrylene	C ₂₀ H ₁₂	199-54-2	382.2
benz[<i>e</i>]acephenanthrylene	C ₂₀ H ₁₂	205-99-2	332.2
benz[<i>j</i>]aceanthrylene	C ₂₀ H ₁₂	202-33-5	398.0
benz[<i>k</i>]acephenanthrylene	C ₂₀ H ₁₂	212-41-9	384.4
benz[<i>l</i>]aceanthrylene	C ₂₀ H ₁₂	211-91-6	407.1
benz[<i>l</i>]acephenanthrylene	C ₂₀ H ₁₂	95690-49-6	403.0
benz[<i>mno</i>]aceanthrylene	C ₁₈ H ₁₀	203-13-4	420.3
benz[<i>mno</i>]indeno[1,7,6,5- <i>cdef</i>]chrysene	C ₂₄ H ₁₂	96915-21-8	443.9
benz[<i>mno</i>]indeno[5,6,7,1- <i>defg</i>]chrysene	C ₂₄ H ₁₂	96915-20-7	444.6
benzo[2,1- <i>a</i> :3,4- <i>a'</i>]dianthracene	C ₃₀ H ₁₈	188-51-2	536.5

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
benzo[3,4]phenanthro[2,1,10,9,8,7- <i>pqrstuv</i>]pentaphene	C ₃₂ H ₁₆	120836-12-6	509.5
benzo[6,7]phenanthro[4,3- <i>b</i>]chrysene	C ₃₄ H ₂₀	119123-34-1	574.2
benzo[<i>a</i>]coronene	C ₂₈ H ₁₄	190-70-5	371.8
benzo[<i>a</i>]cyclopenta[<i>de</i>]naphthacene	C ₂₄ H ₁₄	908068-87-1	470.7
benzo[<i>a</i>]cyclopenta[<i>fg</i>]naphthacene	C ₂₄ H ₁₄	908069-10-3	479.4
benzo[<i>a</i>]cyclopenta[<i>hi</i>]naphthacene	C ₂₄ H ₁₄	908069-47-6	477.8
benzo[<i>a</i>]cyclopenta[<i>mn</i>]naphthacene	C ₂₄ H ₁₄	908069-02-3	478.6
benzo[<i>a</i>]cyclopenta[<i>op</i>]naphthacene	C ₂₄ H ₁₄	908069-25-0	489.4
benzo[<i>a</i>]heptacene	C ₃₄ H ₂₀	93289-29-3	634.3
benzo[<i>a</i>]hexacene	C ₃₀ H ₁₈	240-04-0	541.9
benzo[<i>a</i>]hexaphene	C ₃₀ H ₁₈	115747-79-0	492.1
benzo[<i>a</i>]naphth[2,1- <i>j</i>]anthracene	C ₂₆ H ₁₆	58029-41-7	428.8
benzo[<i>a</i>]naphthacene	C ₂₂ H ₁₄	226-88-0	362.9
benzo[<i>a</i>]naphtho[1,2,3,4- <i>ghi</i>]perylene	C ₃₀ H ₁₆	120835-76-9	487.8
benzo[<i>a</i>]naphtho[1,2- <i>c</i>]naphthacene	C ₃₀ H ₁₈	115747-45-0	524.7
benzo[<i>a</i>]naphtho[1,2- <i>h</i>]anthracene	C ₂₆ H ₁₆	18429-26-0	427.6
benzo[<i>a</i>]naphtho[1,2- <i>j</i>]naphthacene	C ₃₀ H ₁₈	112498-94-9	509.7
benzo[<i>a</i>]naphtho[1,2- <i>l</i>]naphthacene	C ₃₀ H ₁₈	112498-96-1	486.0
benzo[<i>a</i>]naphtho[2,1,8- <i>cde</i>]perylene	C ₃₀ H ₁₆	120835-66-7	477.7
benzo[<i>a</i>]naphtho[2,1,8- <i>hij</i>]naphthacene	C ₂₈ H ₁₆	190-05-6	431.1
benzo[<i>a</i>]naphtho[2,1,8- <i>lmn</i>]perylene	C ₃₀ H ₁₆	120835-71-4	503.3
benzo[<i>a</i>]naphtho[2,1- <i>j</i>]naphthacene	C ₃₀ H ₁₈	112498-97-2	485.5
benzo[<i>a</i>]naphtho[2,1- <i>l</i>]naphthacene	C ₃₀ H ₁₈	115747-87-0	509.7
benzo[<i>a</i>]naphtho[7,8,1,2,3- <i>pqrst</i>]pentaphene	C ₃₀ H ₁₆	120835-78-1	480.6
benzo[<i>a</i>]naphtho[8,1,2- <i>cde</i>]naphthacene	C ₂₈ H ₁₆	192-70-1	443.5
benzo[<i>a</i>]naphtho[8,1,2- <i>klm</i>]perylene	C ₃₀ H ₁₆	120835-73-6	506.6
benzo[<i>a</i>]naphtho[8,1,2- <i>lmn</i>]naphthacene	C ₂₈ H ₁₆	190-01-2	432.6
benzo[<i>a</i>]pentacene	C ₂₆ H ₁₆	239-98-5	451.2
benzo[<i>a</i>]pentaphene	C ₂₆ H ₁₆	7689-57-8	408.2
benzo[<i>a</i>]perylene	C ₂₄ H ₁₄	191-85-5	428.0
benzo[<i>a</i>]picene	C ₂₆ H ₁₆	58029-45-1	428.5

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
benzo[<i>a</i>]pyranthrene	C ₃₄ H ₁₈	191-12-8	523.0
benzo[<i>bc</i>]naphtho[1,2,3- <i>ef</i>]coronene	C ₃₄ H ₁₆	128345-72-2	535.3
benzo[<i>bc</i>]naphtho[3,2,1- <i>ef</i>]coronene	C ₃₄ H ₁₆	128345-69-7	494.0
benzo[<i>b</i>]chrysene	C ₂₂ H ₁₄	214-17-5	347.0
benzo[<i>b</i>]cyclopenta[<i>hi</i>]chrysene	C ₂₄ H ₁₄	908069-32-9	460.4
benzo[<i>b</i>]cyclopenta[<i>qr</i>]chrysene	C ₂₄ H ₁₄	777080-22-5	459.1
benzo[<i>b</i>]naphtho[1,2,3,4- <i>pqr</i>]perylene	C ₃₀ H ₁₆	53156-62-0	477.7
benzo[<i>b</i>]naphtho[1,2- <i>k</i>]chrysene	C ₃₀ H ₁₈	214-15-3	480.9
benzo[<i>b</i>]naphtho[1,2- <i>l</i>]chrysene	C ₃₀ H ₁₈	115747-90-5	505.8
benzo[<i>b</i>]naphtho[2,1- <i>g</i>]chrysene	C ₃₀ H ₁₈	115747-69-8	540.8
benzo[<i>b</i>]naphtho[2,1- <i>k</i>]chrysene	C ₃₀ H ₁₈	115747-91-6	482.1
benzo[<i>b</i>]naphtho[2,1- <i>p</i>]chrysene	C ₃₀ H ₁₈	115747-67-6	538.0
benzo[<i>b</i>]naphtho[2,3- <i>g</i>]chrysene	C ₃₀ H ₁₈	115747-65-4	518.8
benzo[<i>b</i>]naphtho[2,3- <i>l</i>]chrysene	C ₃₀ H ₁₈	115747-71-2	512.6
benzo[<i>b</i>]naphtho[8,1,2- <i>pqr</i>]chrysene	C ₂₈ H ₁₆	137593-96-5	459.7
benzo[<i>b</i>]perylene	C ₂₄ H ₁₄	197-70-6	384.3
benzo[<i>b</i>]picene	C ₂₆ H ₁₆	217-42-5	413.9
benzo[<i>cd</i>]naphtho[3,2,1,8- <i>pqra</i>]perylene	C ₂₈ H ₁₄	6208-20-4	404.5
benzo[<i>c</i>]chrysene	C ₂₂ H ₁₄	194-69-4	362.2
benzo[<i>c</i>]cyclopenta[<i>hi</i>]chrysene	C ₂₄ H ₁₄	908068-67-7	474.4
benzo[<i>c</i>]cyclopenta[<i>qr</i>]chrysene	C ₂₄ H ₁₄	908068-51-9	464.2
benzo[<i>c</i>]hexaphene	C ₃₀ H ₁₈	115747-92-7	491.8
benzo[<i>c</i>]naphtho[1,2- <i>l</i>]chrysene	C ₃₀ H ₁₈	115747-52-9	529.0
benzo[<i>c</i>]naphtho[2,1- <i>m</i>]pentaphene	C ₃₄ H ₂₀	119000-41-8	534.6
benzo[<i>c</i>]naphtho[2,1- <i>p</i>]chrysene	C ₃₀ H ₁₈	27798-46-5	559.1
benzo[<i>c</i>]naphtho[2,3- <i>l</i>]chrysene	C ₃₀ H ₁₈	115747-44-9	536.7
benzo[<i>c</i>]naphtho[7,8,1,2,3- <i>pqrst</i>]pentaphene	C ₃₀ H ₁₆	120835-80-5	455.2
benzo[<i>c</i>]naphtho[8,1,2- <i>ghi</i>]chrysene	C ₂₈ H ₁₆	137570-60-6	474.1
benzo[<i>c</i>]pentaphene	C ₂₆ H ₁₆	222-54-8	407.7
benzo[<i>c</i>]picene	C ₂₆ H ₁₆	217-37-8	403.8
benzo[<i>def</i>]cyclopenta[<i>qr</i>]chrysene	C ₂₂ H ₁₂	153043-82-4	417.4

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
benzo[<i>def</i>]pyranthrene	C ₃₂ H ₁₆	72986-34-6	486.8
benzo[<i>de</i>]cyclopent[<i>a</i>]anthracene	C ₂₀ H ₁₂	198-46-9	419.6
benzo[<i>de</i>]cyclopent[<i>b</i>]anthracene	C ₂₀ H ₁₂	27706-08-7	417.3
benzo[<i>de</i>]naphtho[2,1,8,7- <i>qrst</i>]pentacene	C ₃₀ H ₁₆	120835-83-8	471.1
benzo[<i>de</i>]naphtho[3,2,1- <i>mn</i>]naphthacene	C ₂₈ H ₁₆	120835-45-2	520.9
benzo[<i>de</i>]naphtho[8,1,2,3- <i>stuv</i>]picene	C ₃₀ H ₁₆	120835-74-7	485.6
benzo[<i>ef</i>]phenaleno[9,1,2- <i>abc</i>]coronene	C ₃₆ H ₁₆	128345-76-6	515.6
benzo[<i>e</i>]phenanthro[1,10,9,8- <i>opqra</i>]perylene	C ₃₂ H ₁₆	120835-99-6	527.8
benzo[<i>e</i>]phenanthro[2,3,4,5- <i>pqrab</i>]perylene	C ₃₂ H ₁₆	120836-06-8	492.8
benzo[<i>e</i>]pyrene	C ₂₀ H ₁₂	192-97-2	289.9
benzo[<i>fg</i>]cyclopent[<i>a</i>]anthracene	C ₂₀ H ₁₂	200-63-5	472.7
benzo[<i>fg</i>]naphtho[1,2,3- <i>op</i>]naphthacene	C ₂₈ H ₁₆	137570-59-3	461.2
benzo[<i>f</i>]picene	C ₂₆ H ₁₆	58029-47-3	434.3
benzo[<i>ghi</i>]cyclopenta[<i>cd</i>]perylene	C ₂₄ H ₁₂	190-88-5	417.2
benzo[<i>ghi</i>]fluoranthene	C ₁₈ H ₁₀	203-12-3	364.8
benzo[<i>ghi</i>]naphtho[2,1- <i>a</i>]perylene	C ₃₀ H ₁₆	120835-59-8	467.1
benzo[<i>ghi</i>]naphtho[2,1- <i>b</i>]perylene	C ₃₀ H ₁₆	120835-63-4	461.7
benzo[<i>ghi</i>]perylene	C ₂₂ H ₁₂	191-24-2	301.2
benzo[<i>g</i>]chrysene	C ₂₂ H ₁₄	196-78-1	368.8
benzo[<i>g</i>]naphtho[2,1- <i>b</i>]chrysene	C ₃₀ H ₁₈	115747-57-4	502.4
benzo[<i>g</i>]naphtho[8,1,2- <i>abc</i>]coronene	C ₃₄ H ₁₆	75449-86-4	464.7
benzo[<i>h</i>]naphtho[1,2,3,4- <i>rst</i>]pentaphene	C ₃₂ H ₁₈	31541-02-3	576.9
benzo[<i>h</i>]naphtho[7,8,1,2,3- <i>pqrst</i>]pentaphene	C ₃₀ H ₁₆	120835-69-0	457.3
benzo[<i>h</i>]pentaphene	C ₂₆ H ₁₆	214-91-5	419.0
benzo[<i>h</i>]phenanthro[2,1,10,9,8,7- <i>pqrstuv</i>]pentaphene	C ₃₂ H ₁₆	120835-96-3	482.8
benzo[<i>ij</i>]naphtho[2,1,8,7- <i>defg</i>]pentaphene	C ₃₀ H ₁₆	105786-27-4	462.8
benzo[<i>j</i>]benzo[2,1- <i>a</i> :3,4- <i>a'</i>]dianthracene	C ₃₄ H ₂₀	122961-15-3	594.8
benzo[<i>j</i>]fluoranthene	C ₂₀ H ₁₂	205-82-3	352.0
benzo[<i>j</i>]naphtho[8,1,2- <i>abc</i>]coronene	C ₃₄ H ₁₆	75459-00-6	469.6
benzo[<i>kl</i>]naphtho[2,1,8,7- <i>defg</i>]pentaphene	C ₃₀ H ₁₆	120835-70-3	501.3
benzo[<i>k</i>]fluoranthene	C ₂₀ H ₁₂	207-08-9	339.0

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
benzo[<i>lmn</i>]naphtho[2,1,8- <i>qra</i>]perylene	C ₂₈ H ₁₄	75449-94-4	397.4
benzo[<i>lm</i>]naphtho[1,8- <i>ab</i>]perylene	C ₃₀ H ₁₆	97938-05-1	502.3
benzo[<i>lm</i>]phenanthro[5,4,3- <i>abcd</i>]perylene	C ₃₂ H ₁₆	109278-08-2	489.3
benzo[<i>l</i>]cyclopenta[<i>cd</i>]pyrene	C ₂₂ H ₁₂	113779-16-1	403.9
benzo[<i>l</i>]naphtho[1,2- <i>b</i>]chrysene	C ₃₀ H ₁₈	115747-42-7	494.8
benzo[<i>l</i>]naphtho[2,1- <i>b</i>]chrysene	C ₃₀ H ₁₈	115747-53-0	496.6
benzo[<i>mno</i>]naphtho[1,2- <i>c</i>]chrysene	C ₂₈ H ₁₆	120835-49-6	453.0
benzo[<i>mno</i>]naphtho[2,1- <i>c</i>]chrysene	C ₂₈ H ₁₆	137570-57-1	474.5
benzo[<i>m</i>]naphtho[8,1,2- <i>abc</i>]coronene	C ₃₄ H ₁₆	75449-99-9	465.1
benzo[<i>o</i>]hexaphene	C ₃₀ H ₁₈	115747-76-7	486.9
benzo[<i>pqr</i>]dinaphtho[8,1,2- <i>bcd</i> :2',1',8'- <i>lmn</i>]perylene	C ₃₄ H ₁₆	188-11-4	465.5
benzo[<i>pqr</i>]naphtho[1,2- <i>b</i>]perylene	C ₃₀ H ₁₆	120835-57-6	466.4
benzo[<i>pqr</i>]naphtho[2,1,8- <i>def</i>]picene	C ₃₀ H ₁₆	100684-90-0	471.1
benzo[<i>pqr</i>]naphtho[2,1- <i>b</i>]perylene	C ₃₀ H ₁₆	120835-56-5	467.1
benzo[<i>pqr</i>]naphtho[8,1,2- <i>bcd</i>]perylene	C ₂₈ H ₁₄	190-71-6	382.8
benzo[<i>pqr</i>]naphtho[8,1,2- <i>cde</i>]picene	C ₃₀ H ₁₆	111728-58-6	451.8
benzo[<i>pqr</i>]picene	C ₂₄ H ₁₄	189-96-8	359.4
benzo[<i>p</i>]hexaphene	C ₃₀ H ₁₈	222-81-1	519.6
benzo[<i>p</i>]naphtho[1,2- <i>b</i>]chrysene	C ₃₀ H ₁₈	115747-55-2	500.0
benzo[<i>p</i>]naphtho[1,8,7- <i>ghi</i>]chrysene	C ₂₈ H ₁₆	385-14-8	496.6
benzo[<i>p</i>]naphtho[2,1- <i>b</i>]chrysene	C ₃₀ H ₁₈	115747-56-3	500.0
benzo[<i>p</i>]naphtho[8,1,2- <i>abc</i>]coronene	C ₃₄ H ₁₆	75450-00-9	497.4
benzo[<i>qrs</i>]naphtho[3,2,1,8,7- <i>defgh</i>]pyranthrene	C ₃₆ H ₁₆	128345-79-9	547.0
benzo[<i>qr</i>]naphtho[2,1,8,7- <i>defg</i>]pentacene	C ₃₀ H ₁₆	120835-67-8	462.1
benzo[<i>qr</i>]naphtho[2,1,8,7- <i>fghi</i>]pentacene	C ₃₀ H ₁₆	190-87-4	446.1
benzo[<i>qr</i>]naphtho[3,2,1,8- <i>defg</i>]chrysene	C ₂₆ H ₁₄	75459-05-1	388.9
benzo[<i>q</i>]hexaphene	C ₃₀ H ₁₈	115747-74-5	487.4
benzo[<i>rst</i>]dinaphtho[8,1,2- <i>cde</i> :2',1',8'- <i>klm</i>]pentaphene	C ₃₆ H ₁₈	56181-09-0	548.8
benzo[<i>rst</i>]naphtho[2,1,8- <i>fgh</i>]pentaphene	C ₃₀ H ₁₆	120835-64-5	452.6
benzo[<i>rst</i>]naphtho[8,1,2- <i>cde</i>]pentaphene	C ₃₀ H ₁₆	52879-10-4	460.6
benzo[<i>rst</i>]pentaphene	C ₂₄ H ₁₄	189-55-9	366.0

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
benzo[<i>rst</i>]phenanthro[1,10,9- <i>cde</i>]pentaphene	C ₃₄ H ₁₈	190-93-2	552.5
benzo[<i>rst</i>]phenanthro[10,1,2- <i>cde</i>]pentaphene	C ₃₄ H ₁₈	188-84-1	537.3
benzo[<i>rst</i>]pyreno[1,10,9- <i>cde</i>]pentaphene	C ₃₆ H ₁₈	117740-28-0	562.0
benzo[<i>st</i>]naphtho[2,1,8,7- <i>defg</i>]pentacene	C ₃₀ H ₁₆	14258-76-5	445.0
benzo[<i>s</i>]picene	C ₂₆ H ₁₆	31540-94-0	474.5
benzo[<i>tuv</i>]naphtho[2,1- <i>b</i>]picene	C ₃₂ H ₁₈	119123-35-2	499.7
benzo[<i>uv</i>]naphtho[2,1,8,7- <i>defg</i>]pentacene	C ₃₀ H ₁₆	5869-31-8	452.2
benzo[<i>uv</i>]naphtho[2,1,8,7- <i>defg</i>]pentaphene	C ₃₀ H ₁₆	120835-86-1	487.0
benzo[<i>vwz</i>]hexaphene	C ₂₈ H ₁₆	2828-72-0	443.8
chryseno[2,1- <i>b</i>]picene	C ₃₈ H ₂₂	119000-37-2	605.5
cyclopent[<i>b</i>]indeno[4,5- <i>g</i>]phenanthrene	C ₂₄ H ₁₄	72088-81-4	682.6
cyclopent[<i>b</i>]indeno[5,6- <i>g</i>]phenanthrene	C ₂₄ H ₁₄	72088-82-5	727.6
cyclopent[<i>i</i>]indeno[5,6- <i>a</i>]anthracene	C ₂₄ H ₁₄	222-88-8	679.8
cyclopenta[<i>cd</i>]perylene	C ₂₂ H ₁₂	189-01-5	429.5
cyclopenta[<i>cd</i>]pyrene	C ₁₈ H ₁₀	25732-74-5	343.4
cyclopenta[<i>de</i>]naphthacene	C ₂₀ H ₁₂	16683-64-0	425.5
cyclopenta[<i>de</i>]pentacene	C ₂₄ H ₁₄	16683-65-1	515.3
cyclopenta[<i>de</i>]pentaphene	C ₂₄ H ₁₄	908069-18-1	470.2
cyclopenta[<i>de</i>]picene	C ₂₄ H ₁₄	908069-39-6	449.1
cyclopenta[<i>fg</i>]pentacene	C ₂₄ H ₁₄	908069-55-6	512.2
cyclopenta[<i>fg</i>]pentaphene	C ₂₄ H ₁₄	777080-20-3	457.1
cyclopenta[<i>hi</i>]chrysene	C ₂₀ H ₁₂	216-48-8	382.8
cyclopenta[<i>pg</i>]pentaphene	C ₂₄ H ₁₄		479.0
decacyclene	C ₃₆ H ₁₈	191-48-0	730.8
diademane	C ₁₀ H ₁₀	33840-23-2	296.9
dibenz[<i>a,e</i>]aceanthrylene	C ₂₄ H ₁₄	5385-75-1	413.1
dibenz[<i>a,e</i>]acephenanthrylene	C ₂₄ H ₁₄	2997-45-7	416.6
dibenz[<i>a,j</i>]aceanthrylene	C ₂₄ H ₁₄	203-20-3	423.2
dibenz[<i>a,j</i>]anthracene	C ₂₂ H ₁₄	224-41-9	336.3
dibenz[<i>a,k</i>]acephenanthrylene	C ₂₄ H ₁₄	777080-19-0	468.2
dibenz[<i>a,l</i>]aceanthrylene	C ₂₄ H ₁₄	203-07-6	445.6

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
dibenz[<i>e,ghi</i>]indeno[1,2,3,4- <i>pqra</i>]perylene	C ₃₀ H ₁₄	75449-96-6	561.0
dibenz[<i>e,j</i>]aceanthrylene	C ₂₄ H ₁₄	53974-16-6	447.4
dibenz[<i>e,k</i>]acephenanthrylene	C ₂₄ H ₁₄	206-06-4	405.1
dibenz[<i>e,l</i>]aceanthrylene	C ₂₄ H ₁₄	777080-21-4	456.6
dibenzo[<i>a,cd</i>]naphtho[8,1,2,3- <i>fghi</i>]perylene	C ₃₂ H ₁₆	75459-08-4	502.9
dibenzo[<i>a,c</i>]naphthacene	C ₂₆ H ₁₆	216-00-2	431.7
dibenzo[<i>a,c</i>]pentacene	C ₃₀ H ₁₈	216-08-0	520.4
dibenzo[<i>a,c</i>]pentaphene	C ₃₀ H ₁₈	115747-37-0	480.0
dibenzo[<i>a,c</i>]picene	C ₃₀ H ₁₈	115747-70-1	499.8
dibenzo[<i>a,c</i>]tetraphene	C ₂₆ H ₁₆	53156-67-5	446.0
dibenzo[<i>a,d</i>]coronene	C ₃₂ H ₁₆	120835-89-4	475.5
dibenzo[<i>a,f</i>]perylene	C ₂₈ H ₁₆	191-29-7	555.4
dibenzo[<i>a,f</i>]picene	C ₃₀ H ₁₈	115747-36-9	527.9
dibenzo[<i>a,ghi</i>]naphtho[2,1,8- <i>cde</i>]perylene	C ₃₂ H ₁₆	57789-81-8	491.2
dibenzo[<i>a,ghi</i>]naphtho[2,1,8- <i>lmn</i>]perylene	C ₃₂ H ₁₆	120836-04-6	501.6
dibenzo[<i>a,ghi</i>]naphtho[8,1,2- <i>klm</i>]perylene	C ₃₂ H ₁₆	120836-03-5	487.4
dibenzo[<i>a,ghi</i>]perylene	C ₂₆ H ₁₄	6596-37-8	405.4
dibenzo[<i>a,g</i>]coronene	C ₃₂ H ₁₆	190-66-9	446.0
dibenzo[<i>a,h</i>]pentaphene	C ₃₀ H ₁₈	115747-38-1	478.2
dibenzo[<i>a,j</i>]coronene	C ₃₂ H ₁₆	190-72-7	449.9
dibenzo[<i>a,j</i>]naphthacene	C ₂₆ H ₁₆	227-04-3	415.1
dibenzo[<i>a,j</i>]perylene	C ₂₈ H ₁₆	191-87-7	553.0
dibenzo[<i>a,j</i>]picene	C ₃₀ H ₁₈	115747-54-1	521.6
dibenzo[<i>a,l</i>]naphthacene	C ₂₆ H ₁₆	226-86-8	416.2
dibenzo[<i>a,l</i>]pentacene	C ₃₀ H ₁₈	227-09-8	503.1
dibenzo[<i>a,m</i>]pentaphene	C ₃₀ H ₁₈	115747-83-6	466.1
dibenzo[<i>a,n</i>]pentacene	C ₃₀ H ₁₈	227-07-6	503.2
dibenzo[<i>a,n</i>]perylene	C ₂₈ H ₁₆	191-81-1	489.9
dibenzo[<i>a,n</i>]picene	C ₃₀ H ₁₈	115747-62-1	504.5
dibenzo[<i>a,o</i>]pentaphene	C ₃₀ H ₁₈	115747-60-9	467.6
dibenzo[<i>a,o</i>]perylene	C ₂₈ H ₁₆	190-36-3	532.9

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
dibenzo[<i>a,o</i>]picene	C ₃₀ H ₁₈	115747-93-8	517.2
dibenzo[<i>a,pqr</i>]picene	C ₂₈ H ₁₆	120835-40-7	452.2
dibenzo[<i>a,rst</i>]naphtho[8,1,2- <i>cde</i>]pentaphene	C ₃₄ H ₁₈	191-46-8	554.6
dibenzo[<i>a,rst</i>]pentaphene	C ₂₈ H ₁₆	120835-51-0	455.0
dibenzo[<i>bc,ef</i>]coronene	C ₃₀ H ₁₄	190-31-8	427.7
dibenzo[<i>bc,kl</i>]coronene	C ₃₀ H ₁₄	190-55-6	445.2
dibenzo[<i>b,def</i>]chrysene	C ₂₄ H ₁₄	189-64-0	375.6
dibenzo[<i>b,f</i>]picene	C ₃₀ H ₁₈	115747-68-7	505.9
dibenzo[<i>b,ghi</i>]perylene	C ₂₆ H ₁₄	5869-30-7	373.1
dibenzo[<i>b,g</i>]phenanthrene	C ₂₂ H ₁₄	195-06-2	371.5
dibenzo[<i>b,j</i>]picene	C ₃₀ H ₁₈	115747-48-3	509.3
dibenzo[<i>b,k</i>]chrysene	C ₂₆ H ₁₆	217-54-9	425.4
dibenzo[<i>b,l</i>]chrysene	C ₂₆ H ₁₆	58029-38-2	438.0
dibenzo[<i>b,m</i>]picene	C ₃₀ H ₁₈	82628-46-4	480.8
dibenzo[<i>b,n</i>]picene	C ₃₀ H ₁₈	213-44-5	489.0
dibenzo[<i>b,pqr</i>]perylene	C ₂₆ H ₁₄	190-95-4	373.7
dibenzo[<i>b,p</i>]chrysene	C ₂₆ H ₁₆	58029-42-8	441.0
dibenzo[<i>b,qr</i>]naphtho[3,2,1,8- <i>defg</i>]chrysene	C ₃₀ H ₁₆	120835-61-2	456.1
dibenzo[<i>b,s</i>]picene	C ₃₀ H ₁₈	115747-88-1	550.9
dibenzo[<i>b,tuv</i>]naphtho[2,1- <i>m</i>]picene	C ₃₆ H ₂₀	13354-54-6	572.3
dibenzo[<i>b,tuv</i>]picene	C ₂₈ H ₁₆	189-18-4	438.0
dibenzo[<i>cd,k</i>]naphtho[3,2,1,8- <i>pqra</i>]perylene	C ₃₂ H ₁₆	120836-02-4	485.6
dibenzo[<i>cd,lm</i>]perylene	C ₂₆ H ₁₄	188-96-5	385.5
dibenzo[<i>cd,n</i>]naphtho[3,2,1,8- <i>pqra</i>]perylene	C ₃₂ H ₁₆	109278-09-3	475.9
dibenzo[<i>c,g</i>]chrysene	C ₂₆ H ₁₆	53156-66-4	455.0
dibenzo[<i>c,g</i>]phenanthrene	C ₂₂ H ₁₄	188-52-3	385.5
dibenzo[<i>c,hi</i>]naphtho[3,2,1,8- <i>mno</i>]chrysene	C ₃₀ H ₁₆	120835-72-5	484.6
dibenzo[<i>c,h</i>]pentaphene	C ₃₀ H ₁₈	115747-39-2	478.1
dibenzo[<i>c,i</i>]cyclopenta[<i>a</i>]fluorene	C ₂₄ H ₁₄	63218-07-5	638.2
dibenzo[<i>c,l</i>]chrysene	C ₂₆ H ₁₆	42850-69-1	461.7
dibenzo[<i>c,mno</i>]chrysene	C ₂₄ H ₁₄	196-28-1	383.9

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
dibenzo[<i>c,m</i>]pentaphene	C ₃₀ H ₁₈	222-51-5	465.8
dibenzo[<i>c,m</i>]picene	C ₃₀ H ₁₈	13109-47-2	469.7
dibenzo[<i>c,pqr</i>]picene	C ₂₈ H ₁₆	120835-44-1	427.6
dibenzo[<i>c,p</i>]chrysene	C ₂₆ H ₁₆	196-52-1	464.3
dibenzo[<i>c,rst</i>]pentaphene	C ₂₈ H ₁₆	120835-52-1	430.5
dibenzo[<i>c,s</i>]picene	C ₃₀ H ₁₈	115747-50-7	540.0
dibenzo[<i>def,mno</i>]chrysene	C ₂₂ H ₁₂	191-26-4	323.0
dibenzo[<i>def,mno</i>]cyclopenta[<i>hi</i>]chrysene	C ₂₄ H ₁₂	96915-19-4	441.1
dibenzo[<i>def,p</i>]chrysene	C ₂₄ H ₁₄	191-30-0	393.3
dibenzo[<i>de,ij</i>]naphtho[3,2,1,8,7- <i>rstuv</i>]pentaphene	C ₃₂ H ₁₆	120835-92-9	464.7
dibenzo[<i>de,ij</i>]naphtho[7,8,1,2,3- <i>pqrst</i>]pentaphene	C ₃₂ H ₁₆	120836-00-2	480.8
dibenzo[<i>de,ij</i>]pentaphene	C ₂₈ H ₁₆	120835-46-3	487.8
dibenzo[<i>de,kl</i>]pentaphene	C ₂₈ H ₁₆	83786-06-5	536.1
dibenzo[<i>de,mn</i>]naphthacene	C ₂₄ H ₁₄	214-63-1	421.4
dibenzo[<i>de,mn</i>]naphtho[2,1,8- <i>gra</i>]naphthacene	C ₃₀ H ₁₆	120835-68-9	561.5
dibenzo[<i>de,qr</i>]naphthacene	C ₂₄ H ₁₄	193-09-9	362.6
dibenzo[<i>de,qr</i>]pentacene	C ₂₈ H ₁₆	120835-53-2	483.4
dibenzo[<i>de,st</i>]pentacene	C ₂₈ H ₁₆	14147-38-7	458.5
dibenzo[<i>de,uv</i>]pentacene	C ₂₈ H ₁₆	193-11-3	446.1
dibenzo[<i>de,uv</i>]pentaphene	C ₂₈ H ₁₆	120835-48-5	462.3
dibenzo[<i>ef,hi</i>]naphtho[8,1,2- <i>abc</i>]coronene	C ₃₆ H ₁₆	128395-03-9	513.3
dibenzo[<i>ef,no</i>]naphtho[8,1,2- <i>abc</i>]coronene	C ₃₆ H ₁₆	128515-16-2	527.3
dibenzo[<i>fgh,pqr</i>]trinaphthylene	C ₃₄ H ₁₈	110789-63-4	521.4
dibenzo[<i>fg,ij</i>]naphtho[2,1,8- <i>uva</i>]pentaphene	C ₃₄ H ₁₈	117726-84-8	564.2
dibenzo[<i>fg,ij</i>]naphtho[7,8,1,2,3- <i>pqrst</i>]pentaphene	C ₃₂ H ₁₆	120835-91-8	462.0
dibenzo[<i>fg,ij</i>]pentaphene	C ₂₈ H ₁₆	197-69-3	449.8
dibenzo[<i>fg,ij</i>]phenanthro[2,1,10,9,8,7- <i>pqrstuv</i>]pentaphene	C ₃₄ H ₁₆	187-94-0	486.2
dibenzo[<i>fg,ij</i>]phenanthro[9,10,1,2,3- <i>pqrst</i>]pentaphene	C ₃₆ H ₁₈	188-00-1	534.9
dibenzo[<i>fg,op</i>]naphthacene	C ₂₄ H ₁₄	192-51-8	363.0
dibenzo[<i>fg,qr</i>]pentacene	C ₂₈ H ₁₆	197-74-0	448.2
dibenzo[<i>fg,st</i>]hexacene	C ₃₂ H ₁₈	313-97-3	543.3

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
dibenzo[<i>f,j</i>]naphtho[1,2,3,4- <i>pqr</i>]picene	C ₃₆ H ₂₀	133156-50-0	613.6
dibenzo[<i>f,j</i>]picene	C ₃₀ H ₁₈	188-67-0	524.7
dibenzo[<i>f,pqr</i>]picene	C ₂₈ H ₁₆	120835-42-9	454.3
dibenzo[<i>f,s</i>]picene	C ₃₀ H ₁₈	115747-72-3	544.9
dibenzo[<i>ghi,lm</i>]naphtho[1,8- <i>ab</i>]perylene	C ₃₂ H ₁₆	120864-23-5	522.8
dibenzo[<i>ghi,mno</i>]fluoranthene	C ₂₀ H ₁₀	5821-51-2	498.1
dibenzo[<i>ghi,n</i>]naphtho[8,1,2- <i>bcd</i>]perylene	C ₃₂ H ₁₆	120836-05-7	467.1
dibenzo[<i>g,p</i>]chrysene	C ₂₆ H ₁₆	191-68-4	479.7
dibenzo[<i>hi,kl</i>]naphtho[8,1,2- <i>abc</i>]coronene	C ₃₆ H ₁₆	128345-77-7	540.6
dibenzo[<i>h,rst</i>]pentaphene	C ₂₈ H ₁₆	192-47-2	435.0
dibenzo[<i>ij,rst</i>]naphtho[2,1,8,7- <i>defg</i>]pentaphene	C ₃₂ H ₁₆	75459-09-5	455.4
dibenzo[<i>ij,rst</i>]phenanthro[9,10,1,2- <i>defg</i>]pentaphene	C ₃₆ H ₁₈	313-65-5	527.5
dibenzo[<i>j,lm</i>]naphtho[1,8- <i>ab</i>]perylene	C ₃₄ H ₁₈	93122-98-6	591.0
dibenzo[<i>j,lm</i>]phenanthro[5,4,3- <i>abcd</i>]perylene	C ₃₆ H ₁₈	117726-80-4	575.8
dibenzo[<i>j,l</i>]fluoranthene	C ₂₄ H ₁₄	203-18-9	430.7
dibenzo[<i>kl,no</i>]naphtho[8,1,2- <i>abc</i>]coronene	C ₃₆ H ₁₆	128345-75-5	509.4
dibenzo[<i>kl,rst</i>]naphtho[2,1,8,7- <i>defg</i>]pentaphene	C ₃₂ H ₁₆	120864-22-4	476.6
dibenzo[<i>mn,qr</i>]fluoreno[2,1,9,8,7- <i>defghi</i>]naphthacene	C ₃₀ H ₁₄	76759-99-4	551.2
dibenzo[<i>pq,uv</i>]pentaphene	C ₂₈ H ₁₆	137593-97-6	569.1
dibenzo[<i>q,vwx</i>]hexaphene	C ₃₂ H ₁₈	119000-39-4	501.3
dibenzo[<i>rs,vwx</i>]naphtho[2,1,8,7- <i>klmn</i>]hexaphene	C ₃₆ H ₁₈	117726-81-5	564.5
dicyclopenta[<i>a,c</i>]naphthacene	C ₂₄ H ₁₄	15209-78-6	620.0
dicyclopenta[<i>a,j</i>]coronene	C ₃₀ H ₁₄	90207-46-8	710.9
diindeno[1,2,3- <i>cd</i> :1', <i>d'</i> ,3'- <i>jk</i>]pyrene	C ₂₈ H ₁₄	191-23-1	509.1
dinaphth[1,2- <i>a</i> :1',2'- <i>h</i>]anthracene	C ₃₀ H ₁₈	20495-15-2	525.3
dinaphth[1,2- <i>a</i> :2',1'- <i>j</i>]anthracene	C ₃₀ H ₁₈	68171-26-6	522.9
dinaphtho[1,2,3- <i>fg</i> :1',2',3'- <i>qr</i>]pentacene	C ₃₆ H ₂₀	36474-85-8	636.4
dinaphtho[1,2,3- <i>fg</i> :3',2',1'- <i>qr</i>]pentacene	C ₃₆ H ₂₀	128720-98-9	645.7
dinaphtho[1,2- <i>b</i> :1',2'- <i>k</i>]chrysene	C ₃₄ H ₂₀	214-13-1	537.8
dinaphtho[1,2- <i>b</i> :2',1'- <i>n</i>]perylene	C ₃₆ H ₂₀	197-67-1	585.0
dinaphtho[1,8- <i>ab</i> :8',1',2',3'- <i>fghi</i>]perylene	C ₃₂ H ₁₆	120835-95-2	528.7

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
dinaphtho[1,8- <i>bc</i> :1',8'- <i>mn</i>]picene	C ₃₆ H ₂₀	128721-02-8	726.5
dinaphtho[2,1,8,7- <i>defg</i> :2',1',8',7'- <i>ijkl</i>]pentaphene	C ₃₂ H ₁₆	188-90-9	475.9
dinaphtho[2,1,8,7- <i>defg</i> :2',1',8',7'- <i>opqr</i>]pentacene	C ₃₂ H ₁₆	188-91-0	473.1
dinaphtho[2,1,8,7- <i>defg</i> :2',1',8',7'- <i>qrst</i>]pentacene	C ₃₂ H ₁₆	120835-94-1	457.2
dinaphtho[2,1,8- <i>fgh</i> :3',2',1',8',7'- <i>rstuv</i>]pentaphene	C ₃₂ H ₁₆	120835-93-0	472.0
dinaphtho[2,1,8- <i>fgh</i> :7',8',1',2',3'- <i>pqrst</i>]pentaphene	C ₃₂ H ₁₆	120835-98-5	471.8
dinaphtho[2,1,8- <i>jkl</i> :2',1',8'- <i>uva</i>]pentacene	C ₃₄ H ₁₈	123795-83-5	527.7
dinaphtho[2,1- <i>a</i> :1',2'- <i>l</i>]naphthacene	C ₃₄ H ₂₀	126762-84-3	557.9
dinaphtho[2,1- <i>a</i> :2',1'- <i>j</i>]naphthacene	C ₃₄ H ₂₀	119000-43-0	555.9
dinaphtho[2,1- <i>c</i> :1',2'- <i>g</i>]phenanthrene	C ₃₀ H ₁₈	16914-68-4	562.0
dinaphtho[2,3- <i>c</i> :2',3'- <i>m</i>]pentaphene	C ₃₈ H ₂₂	133979-16-5	612.0
dinaphtho[3,2,1- <i>fg</i> :1',2',3'- <i>ij</i>]pentaphene	C ₃₆ H ₂₀	128720-99-0	650.0
dinaphtho[3,2,1- <i>fg</i> :3',2',1'- <i>qr</i>]pentacene	C ₃₆ H ₂₀	128721-00-6	643.6
dinaphtho[8,1,2- <i>abc</i> :2',1',8'- <i>efg</i>]coronene	C ₃₆ H ₁₆	122677-68-3	487.7
dinaphtho[8,1,2- <i>abc</i> :2',1',8'- <i>hij</i>]coronene	C ₃₆ H ₁₆	128345-74-4	494.2
dinaphtho[8,1,2- <i>abc</i> :2',1',8'- <i>klm</i>]coronene	C ₃₆ H ₁₆	53086-28-5	483.7
dinaphtho[8,1,2- <i>abc</i> :2',1',8'- <i>nop</i>]coronene	C ₃₆ H ₁₆	128395-02-8	518.3
dinaphtho[8,1,2- <i>abc</i> :8',1',2'- <i>ghi</i>]coronene	C ₃₆ H ₁₆	75459-02-8	484.0
dinaphtho[8,1,2- <i>abc</i> :8',1',2'- <i>jkl</i>]coronene	C ₃₆ H ₁₆	190-47-6	492.5
dinaphtho[8,1,2- <i>cde</i> :7',8',1',2',3'- <i>pqrst</i>]pentaphene	C ₃₂ H ₁₆	120835-97-4	485.5
dinaphtho[8,1,2- <i>lmn</i> :2',1',8'- <i>gra</i>]naphthacene	C ₃₀ H ₁₆	58052-99-6	478.2
diphenanthro[3,4- <i>c</i> :4',3'- <i>g</i>]phenanthrene	C ₃₈ H ₂₂	20495-14-1	745.2
fluorantheno[8,9- <i>b</i>]triphenylene	C ₃₂ H ₁₈	24754-03-8	544.1
fluoreno[2,1- <i>a</i>]fluorene	C ₂₄ H ₁₄	221-15-8	574.2
fluoreno[2,3- <i>a</i>]fluorene	C ₂₄ H ₁₄	223-66-5	556.6
fluoreno[3,2,1,9- <i>defg</i>]chrysene	C ₂₆ H ₁₄	192-35-8	438.9
fluoreno[3,2- <i>b</i>]fluorene	C ₂₄ H ₁₄	102634-40-2	536.8
fluoreno[3,4- <i>b</i>]fluorene	C ₂₄ H ₁₄	198-93-6	554.7
fluoreno[4,3,2- <i>de</i>]anthracene	C ₂₄ H ₁₄	195-88-0	533.0
fluoreno[4,3- <i>c</i>]fluorene	C ₂₄ H ₁₄	131238-65-8	565.7
fluoreno[9,1- <i>ab</i>]triphenylene	C ₂₈ H ₁₆	136276-45-4	514.5

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
heptacene	C ₃₀ H ₁₈	258-38-8	586.9
heptalene	C ₁₂ H ₁₀	257-24-9	411.7
heptaphene	C ₃₀ H ₁₈	222-75-3	514.2
hexacene	C ₂₆ H ₁₆	258-31-1	493.7
hexaphene	C ₂₆ H ₁₆	222-78-6	432.6
indeno[1,2,3- <i>cd</i>]fluoranthene	C ₂₂ H ₁₂	193-43-1	453.8
indeno[1,2,3- <i>cd</i>]perylene	C ₂₆ H ₁₄	101686-49-1	448.8
indeno[1,2,3- <i>cd</i>]pyrene	C ₂₂ H ₁₂	193-39-5	360.6
indeno[1,2,3- <i>de</i>]naphthacene	C ₂₄ H ₁₄	314-51-2	450.2
indeno[1,2,3- <i>fg</i>]naphthacene	C ₂₄ H ₁₄	203-11-2	456.1
indeno[1,2,3- <i>hi</i>]chrysene	C ₂₄ H ₁₄	111189-32-3	402.2
indeno[1,2- <i>a</i>]phenalene	C ₂₀ H ₁₂	198-19-6	449.2
indeno[1,7,6,5- <i>cdef</i>]chrysene	C ₂₂ H ₁₂	153043-81-3	415.2
indeno[1,7- <i>ab</i>]chrysene	C ₂₄ H ₁₄	148292-86-8	468.4
indeno[1,7- <i>ab</i>]pyrene	C ₂₂ H ₁₂	196-77-0	404.2
indeno[1,7- <i>ab</i>]triphenylene	C ₂₄ H ₁₄	908068-20-2	479.9
indeno[2,1- <i>a</i>]phenalene	C ₂₀ H ₁₂	200-71-5	376.9
indeno[3,2,1,7- <i>defg</i>]chrysene	C ₂₂ H ₁₂	668-30-4	413.5
indeno[4,3,2,1- <i>cdef</i>]chrysene	C ₂₂ H ₁₂	203-25-8	417.2
indeno[5,6,7,1- <i>defg</i>]chrysene	C ₂₂ H ₁₂	181270-04-2	414.9
indeno[5,6,7,1- <i>pqra</i>]perylene	C ₂₄ H ₁₂	96915-18-3	419.8
indeno[6,7,1,2- <i>defg</i>]naphthacene	C ₂₂ H ₁₂	777080-15-6	501.0
indeno[7,1- <i>ab</i>]naphthacene	C ₂₄ H ₁₄	16683-71-9	467.5
indeno[7,1- <i>ab</i>]triphenylene	C ₂₄ H ₁₄		480.0
indeno[7,1- <i>bc</i>]chrysene	C ₂₄ H ₁₄	777080-23-6	477.7
naphth[1',2':5,6]indeno[1,2,3- <i>cd</i>]pyrene	C ₃₀ H ₁₆	106404-28-8	485.5
naphth[1,2- <i>a</i>]aceanthrylene	C ₂₄ H ₁₄	908069-62-5	459.9
naphth[1,2- <i>a</i>]acephenanthrylene	C ₂₄ H ₁₄	777080-18-9	486.6
naphth[1,2- <i>e</i>]acephenanthrylene	C ₂₄ H ₁₄	5385-22-8	405.8
naphth[1,2- <i>j</i>]aceanthrylene	C ₂₄ H ₁₄	908068-59-7	492.3
naphth[1,2- <i>k</i>]acephenanthrylene	C ₂₄ H ₁₄	201-27-4	442.6

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
naphth[2',1':4,5]indeno[1,2,3- <i>cd</i>]pyrene	C ₃₀ H ₁₆	106404-29-9	514.5
naphth[2,1- <i>a</i>]aceanthrylene	C ₂₄ H ₁₄	75519-75-4	439.4
naphth[2,1- <i>e</i>]aceanthrylene	C ₂₄ H ₁₄	908068-35-9	479.3
naphth[2,1- <i>e</i>]acephenanthrylene	C ₂₄ H ₁₄		406.3
naphth[2,1- <i>k</i>]acephenanthrylene	C ₂₄ H ₁₄	908068-94-0	443.2
naphth[2,1- <i>l</i>]aceanthrylene	C ₂₄ H ₁₄	908068-43-9	501.9
naphth[2,1- <i>l</i>]acephenanthrylene	C ₂₄ H ₁₄	908068-27-9	493.9
naphth[2,3- <i>a</i>]aceanthrylene	C ₂₄ H ₁₄	84030-79-5	424.5
naphth[2,3- <i>e</i>]acephenanthrylene	C ₂₄ H ₁₄	205-97-0	393.6
naphth[2,3- <i>l</i>]acephenanthrylene	C ₂₄ H ₁₄	908068-73-5	479.7
naphthaceno[2,1,12,11- <i>opqra</i>]naphthacene	C ₃₀ H ₁₆	188-42-1	491.2
naphtho[1,2,3,4- <i>def</i>]chrysene	C ₂₄ H ₁₄	192-65-4	363.9
naphtho[1,2,3,4- <i>ghi</i>]perylene	C ₂₆ H ₁₄	190-84-1	382.0
naphtho[1,2,3,4- <i>rst</i>]pentaphene	C ₂₈ H ₁₆	191-20-8	505.1
naphtho[1,2- <i>a</i>]coronene	C ₃₂ H ₁₆	120835-90-7	464.8
naphtho[1,2- <i>a</i>]naphthacene	C ₂₆ H ₁₆	58029-39-3	456.9
naphtho[1,2- <i>a</i>]pentacene	C ₃₀ H ₁₈	115791-74-7	546.2
naphtho[1,2- <i>a</i>]pentaphene	C ₃₀ H ₁₈	115747-85-8	501.1
naphtho[1,2- <i>b</i>]chrysene	C ₂₆ H ₁₆	220-77-9	404.3
naphtho[1,2- <i>b</i>]perylene	C ₂₈ H ₁₆	120835-41-8	451.3
naphtho[1,2- <i>b</i>]picene	C ₃₀ H ₁₈	115747-82-5	471.2
naphtho[1,2- <i>b</i>]triphenylene	C ₂₆ H ₁₆	215-26-9	405.8
naphtho[1,2- <i>c</i>]chrysene	C ₂₆ H ₁₆	58029-46-2	429.7
naphtho[1,2- <i>c</i>]pentaphene	C ₃₀ H ₁₈	115747-80-3	476.5
naphtho[1,2- <i>f</i>]picene	C ₃₀ H ₁₈	115747-49-4	528.9
naphtho[1,2- <i>g</i>]chrysene	C ₂₆ H ₁₆	191-67-3	460.3
naphtho[1,2- <i>h</i>]pentaphene	C ₃₀ H ₁₈	115747-64-3	511.4
naphtho[1,2- <i>j</i>]fluoranthene	C ₂₄ H ₁₄	908069-85-2	440.2
naphtho[1,2- <i>k</i>]fluoranthene	C ₂₄ H ₁₄	238-04-0	402.2
naphtho[2,1,8- <i>def</i>]picene	C ₂₈ H ₁₆	120835-39-4	450.9
naphtho[2,1,8- <i>fgh</i>]pentaphene	C ₂₈ H ₁₆	19301-88-3	435.6

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
naphtho[2,1,8- <i>gra</i>]naphthacene	C ₂₄ H ₁₄	196-42-9	376.5
naphtho[2,1,8- <i>uva</i>]pentacene	C ₂₈ H ₁₆	196-45-2	463.6
naphtho[2,1,8- <i>uva</i>]pentaphene	C ₂₈ H ₁₆	121159-18-0	457.4
naphtho[2,1,8- <i>yz</i> a]hexacene	C ₃₂ H ₁₈	196-46-3	553.0
naphtho[2,1- <i>a</i>]naphthacene	C ₂₆ H ₁₆	220-82-6	434.0
naphtho[2,1- <i>a</i>]pentaphene	C ₃₀ H ₁₈	115747-86-9	478.0
naphtho[2,1- <i>a</i>]picene	C ₃₀ H ₁₈	115747-51-8	495.4
naphtho[2,1- <i>b</i>]chrysene	C ₂₆ H ₁₆	58029-43-9	404.9
naphtho[2,1- <i>b</i>]fluoranthene	C ₂₄ H ₁₄	40563-35-7	422.7
naphtho[2,1- <i>b</i>]perylene	C ₂₈ H ₁₆	120835-43-0	474.0
naphtho[2,1- <i>b</i>]picene	C ₃₀ H ₁₈	115747-81-4	470.2
naphtho[2,1- <i>c</i> :7,8- <i>c'</i>]diphenanthrene	C ₃₄ H ₂₀	20495-12-9	654.3
naphtho[2,1- <i>c</i>]chrysene	C ₂₆ H ₁₆	58029-44-0	450.9
naphtho[2,1- <i>c</i>]pentaphene	C ₃₀ H ₁₈	115791-75-8	500.5
naphtho[2,1- <i>c</i>]picene	C ₃₀ H ₁₈	115747-43-8	494.7
naphtho[2,1- <i>j</i>]fluoranthene	C ₂₄ H ₁₄		415.7
naphtho[2,3- <i>a</i>]coronene	C ₃₂ H ₁₆	190-74-9	447.0
naphtho[2,3- <i>a</i>]pentaphene	C ₃₀ H ₁₈	115747-73-4	482.6
naphtho[2,3- <i>a</i>]picene	C ₃₀ H ₁₈	115747-58-5	503.7
naphtho[2,3- <i>b</i>]picene	C ₃₀ H ₁₈	115747-75-6	497.9
naphtho[2,3- <i>c</i>]chrysene	C ₂₆ H ₁₆	58029-37-1	437.1
naphtho[2,3- <i>c</i>]pentaphene	C ₃₀ H ₁₈	222-58-2	481.5
naphtho[2,3- <i>g</i>]chrysene	C ₂₆ H ₁₆	196-64-5	441.3
naphtho[2,3- <i>j</i>]fluoranthene	C ₂₄ H ₁₄	205-83-4	432.7
naphtho[2,3- <i>k</i>]fluoranthene	C ₂₄ H ₁₄	207-18-1	417.2
naphtho[2,3- <i>s</i>]picene	C ₃₀ H ₁₈	115747-66-5	547.6
naphtho[3,2,1,8,7- <i>defgh</i>]pyranthrene	C ₃₄ H ₁₆	128345-71-1	517.8
naphtho[3,2,1,8,7- <i>vwx</i> yz]hexaphene	C ₃₀ H ₁₆	120835-85-0	464.9
naphtho[4,5,6- <i>abc</i>]aceanthrylene	C ₂₂ H ₁₂	777080-16-7	442.6
naphtho[7,8,1,2,3- <i>pqrst</i>]pentaphene	C ₂₆ H ₁₄	120835-55-4	388.9
naphtho[7,8,1,2,3- <i>tu</i> vwx]hexaphene	C ₃₀ H ₁₆	119123-36-3	468.1

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
naphtho[8,1,2- <i>abc</i>]coronene	C ₃₀ H ₁₄	6596-38-9	392.6
naphtho[8,1,2- <i>bcd</i>]perylene	C ₂₆ H ₁₄	188-89-6	396.3
naphtho[8,1,2- <i>cde</i>]pentaphene	C ₂₈ H ₁₆	120835-50-9	434.1
naphtho[8,1,2- <i>ghi</i>]chrysene	C ₂₄ H ₁₄	35699-67-3	385.2
nonacene	C ₃₈ H ₂₂	258-36-6	774.4
octacene	C ₃₄ H ₂₀	258-33-3	680.5
ovalene	C ₃₂ H ₁₄	190-26-1	404.5
pentacene	C ₂₂ H ₁₄	135-48-8	401.3
pentalene	C ₈ H ₆	250-25-9	381.2
pentaleno[1,2- <i>b</i> :4,5- <i>b'</i>]dinaphthalene	C ₂₄ H ₁₄	155121-10-1	493.0
pentaphene	C ₂₂ H ₁₄	222-93-5	349.3
peri-naphthacenonaphthacene	C ₂₈ H ₁₄	180-50-1	433.2
peri-pentacenopentacene	C ₃₄ H ₁₆	74335-56-1	547.3
perylo[3,2,1,12- <i>pqrab</i>]perylene	C ₃₄ H ₁₆	187-95-1	490.9
phenalene	C ₁₃ H ₁₀	203-80-5	205.5
phenanthro[1,10,9,8- <i>opqra</i>]perylene	C ₂₈ H ₁₄	190-39-6	467.0
phenanthro[1,2,3,4- <i>def</i>]chrysene	C ₂₈ H ₁₆	137570-58-2	458.5
phenanthro[1,2,3,4- <i>ghi</i>]perylene	C ₃₀ H ₁₆	120835-58-7	473.4
phenanthro[1,2- <i>a</i>]naphthacene	C ₃₀ H ₁₈	115747-63-2	521.6
phenanthro[1,2- <i>b</i>]chrysene	C ₃₀ H ₁₈	220-78-0	473.6
phenanthro[10,1,2,3- <i>cdef</i>]fluorene	C ₂₂ H ₁₂	189-75-3	471.3
phenanthro[10,1,2- <i>abc</i>]coronene	C ₃₄ H ₁₆	75459-01-7	468.5
phenanthro[2,1,10,9,8,7- <i>pqrstuv</i>]pentaphene	C ₂₈ H ₁₄	4552-79-8	414.5
phenanthro[2,1,10,9,8,7- <i>tuvwxyz</i>]hexaphene	C ₃₂ H ₁₆	120836-17-1	490.0
phenanthro[2,1- <i>b</i>]chrysene	C ₃₀ H ₁₈	62243-32-7	475.7
phenanthro[2,1- <i>f</i>]picene	C ₃₄ H ₂₀	111381-82-9	588.4
phenanthro[2,3,4,5- <i>tuvab</i>]picene	C ₃₀ H ₁₆	120835-81-6	465.0
phenanthro[2,3- <i>c</i>]chrysene	C ₃₀ H ₁₈	115747-61-0	494.9
phenanthro[2,3- <i>g</i>]chrysene	C ₃₀ H ₁₈	115747-40-5	499.6
phenanthro[3,2- <i>g</i>]chrysene	C ₃₀ H ₁₈	115747-41-6	498.7
phenanthro[3,4- <i>a</i>]naphthacene	C ₃₀ H ₁₈	115747-89-2	522.7

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
phenanthro[3,4- <i>b</i>]chrysene	C ₃₀ H ₁₈	115747-84-7	498.1
phenanthro[3,4- <i>b</i>]triphenylene	C ₃₀ H ₁₈	112498-95-0	497.7
phenanthro[3,4- <i>c</i>]chrysene	C ₃₀ H ₁₈	31124-69-3	537.6
phenanthro[3,4- <i>c</i>]phenanthrene	C ₂₆ H ₁₆	187-83-7	471.7
phenanthro[4,3- <i>a</i>]anthracene	C ₂₆ H ₁₆	58029-40-6	461.2
phenanthro[4,3- <i>b</i>]chrysene	C ₃₀ H ₁₈	42851-11-6	497.1
phenanthro[5,4,3,2- <i>abcde</i>]perylene	C ₂₈ H ₁₄	75449-92-2	391.4
phenanthro[9,10,1,2,3- <i>pqrst</i>]pentaphene	C ₃₀ H ₁₆	120835-79-2	456.8
phenanthro[9,10,1- <i>gra</i>]naphthacene	C ₂₈ H ₁₆	120835-54-3	474.5
phenanthro[9,10- <i>a</i>]naphthacene	C ₃₀ H ₁₈	115791-73-6	531.6
phenanthro[9,10- <i>b</i>]chrysene	C ₃₀ H ₁₈	80277-95-8	475.0
phenanthro[9,10- <i>b</i>]triphenylene	C ₃₀ H ₁₈	215-11-2	478.0
picene	C ₂₂ H ₁₄	213-46-7	336.9
pleiadene	C ₁₈ H ₁₂	206-92-8	414.5
pyranthrene	C ₃₀ H ₁₆	191-13-9	458.1
pyreno[1,10,9- <i>abc</i>]coronene	C ₃₆ H ₁₆	75459-04-0	470.7
pyreno[10,1,2- <i>abc</i>]coronene	C ₃₆ H ₁₆	75449-90-0	495.8
pyreno[2,1- <i>b</i>]picene	C ₃₆ H ₂₀	119000-35-0	566.9
pyreno[5,4,3,2,1- <i>pqrst</i>]pentaphene	C ₃₂ H ₁₆	120836-11-5	502.8
rubicene	C ₂₆ H ₁₄	197-61-5	493.4
s-indacene	C ₁₂ H ₈	267-21-0	407.3
tetrabenzo[<i>a,cd,f,lm</i>]perylene	C ₃₄ H ₁₈	109278-10-6	576.0
tetrabenzo[<i>a,cd,j,lm</i>]perylene	C ₃₄ H ₁₈	191-53-7	565.1
tetrabenzo[<i>a,c,hi,mn</i>]naphthacene	C ₃₂ H ₁₈	109587-16-8	492.7
tetrabenzo[<i>a,c,hi,qr</i>]pentacene	C ₃₆ H ₂₀	192-58-5	565.9
tetrabenzo[<i>a,c,j,l</i>]naphthacene	C ₃₄ H ₂₀	215-95-2	555.4
tetrabenzo[<i>a,c,l,n</i>]pentacene	C ₃₈ H ₂₂	216-07-9	640.9
tetrabenzo[<i>a,e,j,o</i>]perylene	C ₃₆ H ₂₀	128721-01-7	725.9
tetrabenzo[<i>a,f,j,o</i>]perylene	C ₃₆ H ₂₀	191-03-7	739.2
tetrabenzo[<i>a,f,k,n</i>]perylene	C ₃₆ H ₂₀	128746-59-8	716.2
tetrabenzo[<i>bc,ef,hi,kl</i>]coronene	C ₃₆ H ₁₆	128366-79-0	514.4

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
tetrabenzo[<i>bc,ef,kl,no</i>]coronene	C ₃₆ H ₁₆	128345-80-2	614.7
tetrabenzo[<i>de,hi,mn,qr</i>]naphthacene	C ₃₀ H ₁₆	385-13-7	513.7
tetrabenzo[<i>de,hi,op,st</i>]pentacene	C ₃₄ H ₁₈	191-79-7	624.9
tetrabenzo[<i>de,h,kl,rst</i>]pentaphene	C ₃₄ H ₁₈	188-13-6	637.8
tetrabenzo[<i>de,jk,op,uv</i>]pentacene	C ₃₄ H ₁₈	109587-17-9	507.4
tetraphenylene	C ₂₄ H ₁₆	212-74-8	438.4
tribenzo[<i>a,cd,lm</i>]perylene	C ₃₀ H ₁₆	92411-20-6	479.8
tribenzo[<i>a,c,j</i>]naphthacene	C ₃₀ H ₁₈	215-96-3	486.2
tribenzo[<i>a,ef,hi</i>]coronene	C ₃₄ H ₁₆	128345-70-0	496.8
tribenzo[<i>a,ef,no</i>]coronene	C ₃₄ H ₁₆	128345-68-6	511.7
tribenzo[<i>a,e,ghi</i>]perylene	C ₃₀ H ₁₆	120835-60-1	475.1
tribenzo[<i>a,f,j</i>]perylene	C ₃₂ H ₁₈	117440-50-3	636.2
tribenzo[<i>a,ghi,k</i>]perylene	C ₃₀ H ₁₆	120835-75-8	475.6
tribenzo[<i>a,hi,kl</i>]coronene	C ₃₄ H ₁₆	128345-67-5	514.7
tribenzo[<i>a,hi,mn</i>]naphthacene	C ₂₈ H ₁₆	54961-30-7	421.2
tribenzo[<i>b,def,p</i>]chrysene	C ₂₈ H ₁₆	66032-75-9	470.6
tribenzo[<i>b,e,ghi</i>]perylene	C ₃₀ H ₁₆	120835-62-3	472.4
tribenzo[<i>b,g,k</i>]chrysene	C ₃₀ H ₁₈	115747-46-1	518.9
tribenzo[<i>b,g,l</i>]chrysene	C ₃₀ H ₁₈	115747-47-2	540.3
tribenzo[<i>b,g,p</i>]chrysene	C ₃₀ H ₁₈	115747-77-8	551.8
tribenzo[<i>b,n,pqr</i>]perylene	C ₃₀ H ₁₆	190-81-8	445.5
tribenzo[<i>c,g,mno</i>]chrysene	C ₂₈ H ₁₆	108650-10-8	477.2
tribenzo[<i>de,ij,rst</i>]pentaphene	C ₃₀ H ₁₆	120835-65-6	466.7
tribenzo[<i>de,kl,rst</i>]pentaphene	C ₃₀ H ₁₆	188-72-7	490.4
tribenzo[<i>fgh,pqr,za1b1</i>]trinaphthylene	C ₃₆ H ₁₈	97269-75-5	520.4
tribenzo[<i>jk,qr,uv</i>]naphtho[2,1,8,7- <i>defg</i>]pentacene	C ₃₆ H ₁₈	117726-82-6	602.8
trinaphthylene	C ₃₀ H ₁₈	196-62-3	489.3
triquinacene	C ₁₀ H ₁₀	6053-74-3	240.0
truxene	C ₂₇ H ₁₈	548-35-6	393.4

Table S3: Prediction (B3LYP, corrected) of enthalpies of formation ($\Delta_f H_{298K}^\circ$, kJ/mol) for non-PAH molecules for which no experimental values are known.

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
1-cyclopropyl-3-methylbenzene	C ₁₀ H ₁₂	19714-73-9	104.4
1-cyclopropyl-4-methylbenzene	C ₁₀ H ₁₂	6921-43-3	108.6
1-ethenyl-2-methylbenzene	C ₉ H ₁₀	611-15-4	124.4
1-ethenyl-3-methylbenzene	C ₉ H ₁₀	100-80-1	110.9
1-ethenyl-4-ethylbenzene	C ₁₀ H ₁₂	3454-07-7	90.9
1-ethenyl-4-methylbenzene	C ₉ H ₁₀	622-97-9	110.2
1-ethylnaphthalene	C ₁₂ H ₁₀	826-74-4	217.8
1-ethylnaphthalene	C ₁₂ H ₁₂	1127-76-0	97.5
1-ethynyl-2-ethenylbenzene	C ₁₀ H ₈	90766-20-4	391.7
1-ethynyl-2-methylbenzene	C ₉ H ₈	766-47-2	281.9
1-ethynyl-3-ethenylbenzene	C ₁₀ H ₈	114292-48-7	398.1
1-ethynyl-3-methylbenzene	C ₉ H ₈	766-82-5	282.8
1-ethynyl-4-ethenylbenzene	C ₁₀ H ₈	2499-64-1	379.1
1-ethynyl-4-ethylbenzene	C ₁₀ H ₁₀	40307-11-7	262.3
1-ethynyl-4-methylbenzene	C ₉ H ₈	766-97-2	281.9
1-ethynylnaphthalene	C ₁₂ H ₈	15727-65-8	380.9
1-ethynylpentalene	C ₁₀ H ₆		605.8
1-fluorochrysene	C ₁₈ H ₁₁ F ₁		85.1
1-fluoronaphthalene	C ₁₀ H ₇ F ₁	321-38-0	-45.3
1-fluoropyrene	C ₁₆ H ₉ F ₁	1691-65-2	35.6
1-methyl-2-propen-2-ylbenzene	C ₁₀ H ₁₂	7399-49-7	93.2
1-methyl-4-propen-3-ylbenzene	C ₁₀ H ₁₂	1195-32-0	100.3
1-methylindan	C ₁₀ H ₁₂	767-58-8	24.0
1-methylindene	C ₁₀ H ₁₀	767-59-9	128.3
1-methylnaphth-2-yl	C ₁₁ H ₉	7419-61-6	363.3
1-methylpentalene	C ₉ H ₈	33131-61-2	339.1
1-phenylethenyl	C ₈ H ₇		342.8
1-phenylethyl	C ₈ H ₉		169.1
1-phenylnaphthalene	C ₁₆ H ₁₂	605-02-7	250.9
1-phenylprop-1-yl	C ₉ H ₁₁	19019-92-2	149.9
1-phenylprop-2-yl	C ₉ H ₁₁		193.9
1-phenylprop-3-yl	C ₉ H ₁₁		208.7
1-phenylpropen-1-yl	C ₉ H ₉		313.7
1-phenylpropen-2-yl	C ₉ H ₉		335.4
1-phenylpropen-3-yl	C ₉ H ₉		230.5
1,2-diethenylbenzene	C ₁₀ H ₁₀	91-14-5	222.6
1,2-diethynylbenzene	C ₁₀ H ₆	21792-52-9	558.3
1,2-dihydronaphthalen-4y-l	C ₁₀ H ₉		370.6
1,2-dimethylnaphthalene	C ₁₂ H ₁₂	573-98-8	91.6
1,2-dimethylpentalene	C ₁₀ H ₁₀		302.7
1,2,3,4-tetrahydro-2-methylnaphthalene	C ₁₁ H ₁₄	3877-19-8	-8.6

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
1,2,3,4-tetrahydro-5-methylnaphthalene	C ₁₁ H ₁₄	2809-64-5	−0.7
1,3-diethenylbenzene	C ₁₀ H ₁₀	108-57-6	209.4
1,3-diethynylbenzene	C ₁₀ H ₆	1785-61-1	555.1
1,3-dimethylnaphthalene	C ₁₂ H ₁₂	575-41-7	80.9
1,3-dimethylpentalene	C ₁₀ H ₁₀	42340-10-3	291.6
1,4-diethenylbenzene	C ₁₀ H ₁₀	105-06-6	207.0
1,4-diethynylbenzene	C ₁₀ H ₆	935-14-8	552.6
1,4-dimethylnaphthalene	C ₁₂ H ₁₂	571-58-4	85.9
1,4-dimethylpentalene	C ₁₀ H ₁₀		297.9
1,5-diethylnaphthalene	C ₁₄ H ₈	67665-34-3	621.7
1,5-dimethylpentalene	C ₁₀ H ₁₀	60212-21-7	299.0
1,6-dimethylnaphthalene	C ₁₂ H ₁₂	575-43-9	81.1
1,6-dimethylpentalene	C ₁₀ H ₁₀		293.6
1,7-dimethylnaphthalene	C ₁₂ H ₁₂	575-37-1	81.4
1,8-diethylnaphthalene	C ₁₄ H ₈	18067-44-2	648.3
2-ethenylnaphthalene	C ₁₂ H ₁₀	827-54-3	205.3
2-ethylnaphthalene	C ₁₂ H ₁₂	939-27-5	89.7
2-ethynylnaphthalene	C ₁₂ H ₈	2949-26-0	378.9
2-ethynylpentalene	C ₁₀ H ₆		604.9
2-fluorofluorene	C ₁₃ H ₉ F ₁	343-43-1	−7.8
2-fluorophenanthrene	C ₁₄ H ₉ F ₁	532-41-1	15.1
(2-methylbut-1-enyl)benzene	C ₁₁ H ₁₄	56253-64-6	66.5
2-methyleneindene	C ₁₀ H ₈	6596-86-7	319.0
2-methylindene	C ₁₀ H ₁₀	2177-47-1	115.6
2-methylpentalene	C ₉ H ₈	42340-22-7	340.2
2-methylphenyl	C ₇ H ₇	22904-44-5	294.2
2-phenylbut-2-yl	C ₁₀ H ₁₃		123.4
2-phenylethyl	C ₈ H ₉	17203-53-1	229.0
2-phenylnaphthalene	C ₁₆ H ₁₂	612-94-2	239.4
2-phenylprop-1-yl	C ₉ H ₁₁		199.6
2-phenylprop-2-yl	C ₉ H ₁₁	16804-70-9	134.1
2-phenylpropen-1-yl	C ₉ H ₉		360.0
2-phenylpropen-3-yl	C ₉ H ₉		263.4
2,2-dimethylindan	C ₁₁ H ₁₄	20836-11-7	−9.6
3-fluorochrysene	C ₁₈ H ₁₁ F ₁	36288-22-9	82.9
3-fluorofluoranthene	C ₁₆ H ₉ F ₁	1691-66-3	92.2
3-fluorophenanthrene	C ₁₄ H ₉ F ₁	440-40-4	14.5
3-methylindene	C ₁₀ H ₁₀	767-60-2	115.9
3-methylpenta-1,2-diene	C ₆ H ₁₀	7417-48-3	112.9
3-methylphenyl	C ₇ H ₇	3474-41-7	294.8
3-phenylpropen-1-yl	C ₉ H ₉		378.6
3-phenylpropen-2-yl	C ₉ H ₉		361.3
3-phenylpropen-3-yl	C ₉ H ₉		230.6
3-phenylpropyn-1-yl	C ₉ H ₇		649.1

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
3-phenylpropyn-3-yl	C ₉ H ₇		409.2
4-fluorophenanthrene	C ₁₄ H ₉ F ₁	521-66-4	23.8
4-methylpenta-1,2-diene	C ₆ H ₁₀	13643-05-5	114.4
4-methylphenyl	C ₇ H ₇	2396-02-3	297.1
4,7-dimethylindan	C ₁₁ H ₁₄		-5.1
5-fluoroacenaphthylene	C ₁₂ H ₇ F ₁	17251-01-6	73.8
5-methylchrysene	C ₁₉ H ₁₄	3697-24-3	274.1
5-methylindan	C ₁₀ H ₁₂	874-35-1	26.5
9-fluorobenzo[<i>k</i>]fluoranthene	C ₂₀ H ₁₁ F ₁	113600-15-0	151.3
azulen-1-yl	C ₁₀ H ₇		544.9
azulen-4-yl	C ₁₀ H ₇		503.2
azulen-5-yl	C ₁₀ H ₇		509.2
azulen-6-yl	C ₁₀ H ₇		510.3
benz-1,2-yn-3-yl	C ₆ H ₃		711.7
benzocyclobut-1-yl	C ₈ H ₇		359.3
benzocyclobut-4-yl	C ₈ H ₇		440.0
benzocyclobuten-1-yl	C ₈ H ₅		665.7
benzocyclobuten-3-yl	C ₈ H ₅		662.1
benzocyclobuten-4-yl	C ₈ H ₅		661.1
benzocycloprop-3-yl	C ₇ H ₅		604.1
benzocycloprop-4-yl	C ₇ H ₅		611.9
benzocyclopropane	C ₇ H ₆	4646-69-9	360.6
benzyl	C ₇ H ₇	2154-56-5	199.3
benzyne	C ₆ H ₄	462-80-6	467.8
(<i>E</i>)-but-1-en-1-ylbenzene	C ₁₀ H ₁₂	1005-64-7	90.4
(<i>E</i>)-but-2-ene	C ₄ H ₈	107-01-7	-13.8
buta-1,2-dien-3-ylbenzene	C ₁₀ H ₁₀	22433-39-2	246.7
buta-1,2-diene	C ₄ H ₆	590-19-2	162.1
(<i>E</i>)-buta-1,3-dien-1-ylbenzene	C ₁₀ H ₁₀		192.2
(<i>Z</i>)-buta-1,3-dien-1-ylbenzene	C ₁₀ H ₁₀	31915-94-3	228.9
buta-1,3-dien-2-ylbenzene	C ₁₀ H ₁₀		215.6
buta-1,3-diene	C ₄ H ₆		122.5
butatriene	C ₄ H ₄	2873-50-9	314.6
cis-decalin	C ₁₀ H ₁₈	493-01-6	-128.7
cyclobuta[<i>e</i>]indan	C ₁₁ H ₁₂	60582-11-8	172.3
cyclobutylbenzene	C ₁₀ H ₁₂	4392-30-7	118.1
cyclopent-1-en-1-ylbenzene	C ₁₁ H ₁₂	825-54-7	120.3
cyclopent-2-en-1-ylbenzene	C ₁₁ H ₁₂	37689-22-8	136.7
cyclopent-3-en-1-ylbenzene	C ₁₁ H ₁₂	39599-89-8	136.7
cyclopentylbenzene	C ₁₁ H ₁₄	700-88-9	26.3
cyclopropa[<i>b</i>]anthracene	C ₁₅ H ₁₀	287-03-6	499.6
cyclopropylbenzene	C ₉ H ₁₀	873-49-4	139.4
hexa-1,2,3-trien-5-yne	C ₆ H ₄	895126-88-2	555.5
(<i>E</i>)-hexa-1,2,4,5-tetraene	C ₆ H ₆	29776-96-3	391.8

Molecule	Formula	CASNO	$\Delta_f H_{298K}^\circ$
hexa-1,5-diyne	C ₆ H ₆	628-16-0	437.7
hexa-2,3-diene	C ₆ H ₁₀	592-49-4	116.1
(<i>E</i>)-hexa-2,3,4-triene	C ₆ H ₈	59660-65-0	248.3
hexapentaene	C ₆ H ₄	13703-38-3	547.3
hexatriyne	C ₆ H ₂	3161-99-7	685.3
indan-1-yl	C ₉ H ₉		196.9
indan-2-yl	C ₉ H ₉		237.1
inden-1-yl	C ₉ H ₇	71551-80-9	271.2
inden-2-yl	C ₉ H ₇		422.8
inden-4-yl	C ₉ H ₇		408.7
inden-5-yl	C ₉ H ₇		408.4
inden-6-yl	C ₉ H ₇		409.1
inden-7-yl	C ₉ H ₇		406.5
isohexyne	C ₆ H ₁₀	7154-75-8	130.2
isopropen-1-ylbenzene	C ₁₀ H ₁₂	768-49-0	83.3
isopropen-3-ylbenzene	C ₁₀ H ₁₂	3290-53-7	94.5
methane	C ₁ H ₄	74-82-8	-79.2
naphth-1-yl	C ₁₀ H ₇	2510-51-2	393.1
naphth-1-ylmethyl	C ₁₁ H ₉	7419-60-5	265.3
naphth-2-yl	C ₁₀ H ₇	10237-50-0	392.7
p-benzyne	C ₆ H ₄	3355-34-8	626.3
pent-1-en-3-yne	C ₅ H ₆	646-05-9	255.0
pent-1-en-4-yne	C ₅ H ₆	871-28-3	288.8
(<i>E</i>)-pent-2-en-2-ylbenzene	C ₁₁ H ₁₄	53172-84-2	69.3
penta-1,2,3-triene	C ₅ H ₆	62018-46-6	280.6
penta-1,2,4-triene	C ₅ H ₆	10563-01-6	252.6
penta-1,2-diene	C ₅ H ₈	591-95-7	143.1
penta-1,3-diyne	C ₅ H ₄	1033-27-7	418.7
penta-1,4-diyne	C ₅ H ₄	24442-69-1	472.0
penta-2,3-diene	C ₅ H ₈	591-96-8	136.2
pentalen-1-yl	C ₈ H ₅		642.8
pentalen-2-yl	C ₈ H ₅		650.8
pentatetraene	C ₅ H ₄	21986-03-8	426.3
propa-1,2-dienylbenzene	C ₉ H ₈	2327-99-3	273.0
propadiene	C ₃ H ₄	463-49-0	188.5
propyn-3-ylbenzene	C ₉ H ₈	10147-11-2	307.4
tert-heptyne	C ₇ H ₁₂	918-82-1	103.4

Table S4: Corrected values of the enthalpy of formation $\Delta_f H_{298K}^\circ$ (kJ/mol) computed using the G3MP2B3 model chemistry for molecules where no experimental data are available.

Name	Formula	CASNO	$\Delta_f H_{298K}^\circ$ (est)	$\Delta_f H_{298K}^\circ$ G3MP2B3 (corr)	residual
<i>Estimated Literature Values</i>					
cyclopropylbenzene	C ₉ H ₁₀	873-49-4	162.0	161.1	−0.9
cyclobutylbenzene	C ₁₀ H ₁₂	4392-30-7	136.0	128.7	−7.3
cyclopentylbenzene	C ₁₁ H ₁₄	700-88-9	32.0 ± 4.4	28.7	−3.3
1-ethylnaphthalene	C ₁₂ H ₁₂	1127-76-0	98.0 ± 5.0	97.1	−0.9
2-ethylnaphthalene	C ₁₂ H ₁₂	939-27-5	98.0 ± 5.0	94.1	−3.9
1,2-dimethylnaphthalene	C ₁₂ H ₁₂	573-98-8	84.6 ± 5.6	90.0	5.4
1,3-dimethylnaphthalene	C ₁₂ H ₁₂	575-41-7	84.6 ± 5.6	82.8	−1.8
1,4-dimethylnaphthalene	C ₁₂ H ₁₂	571-58-4	84.6 ± 5.6	84.7	0.1
1,6-dimethylnaphthalene	C ₁₂ H ₁₂	575-43-9	84.6 ± 5.6	83.1	−1.5
1,7-dimethylnaphthalene	C ₁₂ H ₁₂	575-37-1	84.6 ± 5.6	82.9	−1.7
1-ethenyl-2-methylbenzene	C ₉ H ₁₀	611-15-4	115.6 ± 4.4	125.2	9.6
1-ethenyl-3-methylbenzene	C ₉ H ₁₀	100-80-1	115.6 ± 4.4	115.7	0.1
1-ethenyl-4-methylbenzene	C ₉ H ₁₀	622-97-9	115.6 ± 4.4	113.6	−2.0
1-ethenyl-4-ethylbenzene	C ₁₀ H ₁₂	3454-07-7	96.4 ± 4.9	94.0	−2.4
1-methyl-2-propen-2-ylbenzene	C ₁₀ H ₁₂	7399-49-7	87.9 ± 6.2	89.8	1.9
cyclopent-1-en-1-ylbenzene	C ₁₁ H ₁₂	825-54-7	130.3 ± 6.6	124.0	−6.3
(2-methylbut-1-enyl)benzene	C ₁₁ H ₁₄	56253-64-6	69.0 ± 6.4	69.2	0.2
1,2-Diethenylbenzene	C ₁₀ H ₁₀	91-14-5	213.6 ± 4.8	220.5	6.9
1,3-Diethenylbenzene	C ₁₀ H ₁₀	108-57-6	213.6 ± 4.8	212.4	−1.2
1,4-diethenylbenzene	C ₁₀ H ₁₀	105-06-6	213.6 ± 4.8	211.5	−2.1
1-ethenylnaphthalene	C ₁₂ H ₁₀	826-74-4	215.2 ± 4.9	221.2	6.0
2-ethenylnaphthalene	C ₁₂ H ₁₀	827-54-3	215.2 ± 4.9	210.8	−4.4

Name	Formula	CASNO	$\Delta_f H_{298K}^\circ$ (est)	$\Delta_f H_{298K}^\circ$ G3MP2B3 (corr)	residual
1,2-diethynylbenzene	C ₁₀ H ₆	21792-52-9	536.0 ± 11.0	555.5	19.5
1,3-diethynylbenzene	C ₁₀ H ₆	1785-61-1	536.0 ± 11.0	553.9	17.9
1-ethynynaphthalene	C ₁₂ H ₈	15727-65-8	376.5 ± 8.1	381.5	5.0
1-phenylnaphthalene	C ₁₆ H ₁₂	605-02-7	248.6 ± 5.8	246.4	-2.2
<i>No Literature Values</i>					
1-cyclopropyl-3-methylbenzene	C ₁₀ H ₁₂	19714-73-9		124.9	
1-cyclopropyl-4-methylbenzene	C ₁₀ H ₁₂	6921-43-3		129.2	
1-methyl-3-propen-2-ylbenzene	C ₁₀ H ₁₂	1124-20-5		84.6	
isopropen-1-ylbenzene	C ₁₀ H ₁₂			88.1	
isopropen-3-ylbenzene	C ₁₀ H ₁₂			95.5	
1-methyl-4-propen-3-ylbenzene	C ₁₀ H ₁₂	1195-32-0		100.0	
(E)-but-1-en-1-ylbenzene	C ₁₀ H ₁₂	1005-64-7		97.5	
(E)-pent-2-en-2-ylbenzene	C ₁₁ H ₁₄	53172-84-2		71.6	
cyclopent-2-en-1-ylbenzene	C ₁₁ H ₁₂	37689-22-8		137.5	
cyclopent-3-en-1-ylbenzene	C ₁₁ H ₁₂	39599-89-8		137.6	
(E)-buta-1,3-dien-1-ylbenzene	C ₁₀ H ₁₀	16939-57-4		203.3	
(Z)-buta-1,3-dien-1-ylbenzene	C ₁₀ H ₁₀	16939-57-4		230.2	
buta-1,3-dien-2-ylbenzene	C ₁₀ H ₁₀	2288-18-8		216.5	
buta-1,2-dien-3-ylbenzene	C ₁₀ H ₁₀	22433-39-2		252.4	
buta-1,3-dien-2-ylbenzene	C ₁₀ H ₁₀	2288-18-8		212.4	
1-ethynyl-2-methylbenzene	C ₉ H ₈	766-47-2		282.0	
1-ethynyl-3-methylbenzene	C ₉ H ₈	766-82-5		285.3	
1-ethynyl-4-methylbenzene	C ₉ H ₈	766-97-2		282.8	
1-ethynyl-4-ethylbenzene	C ₁₀ H ₁₀	40307-11-7		263.4	

Name	Formula	CASNO	$\Delta_f H_{298K}^\circ$ (est)	$\Delta_f H_{298K}^\circ$ G3MP2B3 (corr)	residual
1-ethynyl-2-ethenylbenzene	C ₁₀ H ₈			380.7	
1-ethynyl-3-ethenylbenzene	C ₁₀ H ₈			380.4	
1-ethynyl-4-ethenylbenzene	C ₁₀ H ₈			379.6	
2-ethynylnaphthalene	C ₁₂ H ₈	2949-26-0		382.9	
1,4-Diethynylbenzene	C ₁₀ H ₆	935-14-8		552.7	
1,5-diethynylnaphthalene	C ₁₄ H ₈	67665-34-3		612.2	
1,8-diethynylnaphthalene	C ₁₄ H ₈	18067-44-2		636.6	
2-phenylnaphthalene	C ₁₆ H ₁₂	612-94-2		203.2	
diademane	C ₁₀ H ₁₀	33840-23-2		375.5	
1,2,3,4-tetrahydro-2-methylnaphthalene	C ₁₁ H ₁₄			-9.5	
1,2,3,4-tetrahydro-5-methylnaphthalene	C ₁₁ H ₁₄	2809-64-5		-8.8	
aceanthrylene	C ₁₆ H ₁₀	202-03-9		333.0	
acephenanthrene	C ₁₆ H ₁₀	201-06-9		305.1	
as-indacene	C ₁₂ H ₈	210-65-1		425.8	
s-indacene	C ₁₂ H ₈	267-21-0		415.1	
heptalene	C ₁₂ H ₁₀	257-24-9		412.5	
phenalene	C ₁₃ H ₁₀	203-80-5		204.5	
2-methyleneindene	C ₁₀ H ₈			321.3	
pentalene	C ₈ H ₆	250-25-9		371.2	
1-methylpentalene	C ₉ H ₈	33131-61-2		333.4	
1,2-dimethylpentalene	C ₁₀ H ₁₀			297.6	
1,3-dimethylpentalene	C ₁₀ H ₁₀			289.7	
1-ethynylpentalene	C ₁₀ H ₆			598.9	