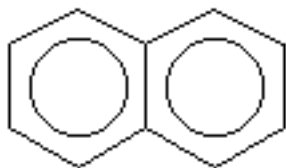


Naphthalene

- **Fórmula:** C₁₀H₈
- **Peso molecular:** 128.17
- **Identificador Químico Internacional de IUPAC:**
 - InChI=1/C10H8/c1-2-6-10-8-4-3-7-9(10)5-1/h1-8H
 - [Download the identifier in a file.](#)
- **Número de registro CAS:** 91-20-3
- **Estructura química:**



Esta estructura está también disponible como [2d Mol file](#) o como [computed 3d Mol file](#).

- **Isotopómeros:**
 - [Naphthalene-d8](#)
- **Otros nombres:** Albocarbon; Dezodorator; Moth flakes; Naphthalin; Naphthaline; Naphthene; Tar camphor; White tar; Camphor tar; Moth balls; Naftalen; NCI-C52904; Mighty 150; Mighty rd1; Napthalene, molten; Rcra waste number U165; UN 1334; UN 2304
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 - [Condensed phase thermochemistry data](#)
 - [Phase change data](#)
 - [Reaction thermochemistry data](#)
 - [Henry's Law data](#)
 - [Ion clustering data](#)
 - [IR Spectrum](#)
 - [Mass Spectrum](#)
 - [UV/Visible Spectrum](#)

- [Gas Chromatography](#)
- **Data at other NIST sites:**
 - [Computational Chemistry Comparison and Benchmark Database \(on SRD web site\)](#)
 - [Gas phase kinetics \(on kinetics web site\)](#)
 - [X-ray Photoelectron Spectroscopy Database \(on SRD web site\)](#)
- **Options:**
 - [Switch to calorie-based units](#)

Gas phase ion energetics data

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Data evaluated as indicated in comments:

HL - E.P. Hunter and S.G. Lias

L - S.G. Lias

Data compiled as indicated in comments:

B - J.E. Bartmess

LL - S.G. Lias and J.F. Liebman

LBLHLM - S.G. Lias, J.E. Bartmess, J.F. Liebman, J.L. Holmes, R.D. Levin, and W.G. Mallard

LLK - S.G. Lias, R.D. Levin, and S.A. Kafafi

RDSH - H.M. Rosenstock, K. Draxl, B.W. Steiner, and J.T. Herron

[View reactions leading to C₁₀H₈⁺ \(ion structure unspecified\)](#)

Quantity	Value	Units	Method	Reference	Comment
IE (evaluated)	8.144 ± 0.001	eV	N/A	N/A	<i>L</i>
Quantity	Value	Units	Method	Reference	Comment
Proton affinity (review)	802.9	kJ/mol	N/A	Hunter and Lias, 1998	<i>HL</i>
Quantity	Value	Units	Method	Reference	Comment
Gas basicity (review)	779.4	kJ/mol	N/A	Hunter and Lias, 1998	<i>HL</i>

Electron affinity determinations

EA (eV)	Method	Reference	Comment
-0.2	LPES	Lyapustina, Xu, et al., 2000	Extrapolated from EAs of solvation series naphthalene-...(H ₂ O) _n ; <i>B</i>
-0.200 ± 0.050	LPES	Schiedt, Knott, et al., 2000	Extrapolated from EAs of (H ₂ O) _n .. naphthalene-. series; <i>B</i>
-0.18	N/A	Song, Han, et al., 2002	Extrapolated from LPES EAs of (naphthalene) _n ; <i>B</i>
-0.1908	ETS	Burrow, Michejda, et al., 1987	The question of whether the naphthalene radical anion is bound or not has not been settled; <i>B</i>
0.140 ± 0.050	ECD	Zlatkis, Lee, et al., 1983	However, see Heinis, Chowdhury, et al., 1993 for a discussion; it may not be bound.; <i>B</i>
<0.134 ± 0.043	ECD	Wojnarovits and Foldiak, 1981	EA is an upper limit: Chen and Wentworth, 1989; <i>B</i>
0.1480 ± 0.0060	ECD	Becker and Chen, 1966	<i>B</i>

Ionization energy determinations

IE (eV)	Method	Reference	Comment
8.12 ± 0.02	TRPI	Gotkis, Oleinikova, et al., 1993	<i>LL</i>
8.1442 ± 0.0009	TE	Cockett, Ozeki, et al., 1993	<i>LL</i>
8.12 ± 0.01	PI	Jochims, Rasekh, et al., 1992	<i>LL</i>
8.14	EI	Stahl and Maquin, 1984	<i>LBLHLM</i>
8.141 ± 0.001	LS	Duncan, Dietz, et al., 1981	<i>LLK</i>
8.08 ± 0.05	EQ	Mautner(Meot-Ner), 1980	<i>LLK</i>
8.15	PE	Schafer, Schweig, et al., 1975	<i>LLK</i>
8.15	PE	Schafer, Schweig, et al., 1973	<i>LLK</i>
8.12	CTS	Pitt, 1973	<i>LLK</i>
8.15	PE	Clark, Brogli, et al., 1972	<i>LLK</i>
8.13	PE	Brundle, Robin, et al., 1972	<i>LLK</i>

8.15	PE	Brogli, Heilbronner, et al., 1972	<i>LLK</i>
8.16 ± 0.03	EI	Johnstone, Mellon, et al., 1970	<i>RDSH</i>
8.11 ± 0.01	PE	Dewar and Worley, 1969	<i>RDSH</i>
8.15 ± 0.01	PI	Yencha and El-Sayed, 1968	<i>RDSH</i>
8.133	S	Kitagawa, 1968	<i>RDSH</i>
8.14	PI	Kitagawa, 1968	<i>RDSH</i>
8.12 ± 0.05	PE	Eland and Danby, 1968	<i>RDSH</i>
8.136 ± 0.005	S	Angus, Christ, et al., 1968	<i>RDSH</i>
8.25 ± 0.01	EI	Bonnier, Gelus, et al., 1965	<i>RDSH</i>
8.15	CTS	Kuroda, 1964	<i>RDSH</i>
8.16	CTS	Briegleb, 1964	<i>RDSH</i>
8.08	CTS	Kinoshita, 1962	<i>RDSH</i>
8.1	PI	Terenin, 1961	<i>RDSH</i>
8.10	CTS	Birks and Stifkin, 1961	<i>RDSH</i>
8.12 ± 0.01	PI	Watanabe, 1957	<i>RDSH</i>
8.14 ± 0.02	PI	Vilesov and Terenin, 1957	<i>RDSH</i>
8.09	PE	Klasinc, Kovac, et al., 1983	Vertical value; <i>LBLHLM</i>
8.15	PE	Kaim, Tesmann, et al., 1980	Vertical value; <i>LLK</i>
8.15 ± 0.02	PE	Schmidt, 1977	Vertical value; <i>LLK</i>
8.18 ± 0.03	PE	Heilbronner, Hoshi, et al., 1976	Vertical value; <i>LLK</i>
8.15	PE	Clar and Schmidt, 1976	Vertical value; <i>LLK</i>
8.31 ± 0.03	PE	Marschner and Goetz, 1974	Vertical value; <i>LLK</i>
8.15	PE	Bock, Wagner, et al., 1972	Vertical value; <i>LLK</i>
8.15	PE	Bock and Wagner, 1972	Vertical value; <i>LLK</i>

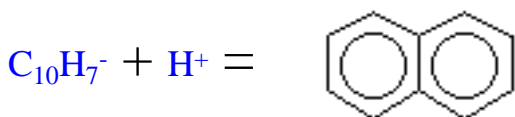
Appearance energy determinations

Ion	AE (eV)	Other Products	Method	Reference	Comment
C_3H_3^+	19.35	?	PI	Jochims, Rasekh, et al., 1993	<i>LL</i>

C_3H_3^+	19.2 ± 0.1	$\text{C}_3\text{H}_3 + \text{C}_4\text{H}_2$	PI	Jochims, Rasekh, et al., 1992	<i>LL</i>
C_4H_2^+	20.7 ± 0.1	$3\text{C}_2\text{H}_2$	PI	Jochims, Rasekh, et al., 1992	<i>LL</i>
C_4H_3^+	22.3 ± 0.1	$2\text{C}_2\text{H}_2 + \text{C}_2\text{H}$	PI	Jochims, Rasekh, et al., 1992	<i>LL</i>
C_4H_4^+	19.4 ± 0.1	$\text{C}_4\text{H}_2 + \text{C}_2\text{H}_2$	PI	Jochims, Rasekh, et al., 1992	<i>LL</i>
C_4H_4^+	19.6 ± 0.20	?	EI	VanBrunt and Wacks, 1964	<i>RDSH</i>
C_5H_3^+	19.74	?	PI	Jochims, Rasekh, et al., 1993	<i>LL</i>
C_5H_3^+	19.7 ± 0.1	$\text{C}_2\text{H}_2 + \text{C}_3\text{H}_3$	PI	Jochims, Rasekh, et al., 1992	<i>LL</i>
C_6H_3^+	20.77 ± 0.01	?	EI	VanBrunt and Wacks, 1964	<i>RDSH</i>
C_6H_4^+	18.7 ± 0.1	$2\text{C}_2\text{H}_2$	PI	Jochims, Rasekh, et al., 1992	<i>LL</i>
C_6H_4^+	18.2 ± 0.15	?	EI	VanBrunt and Wacks, 1964	<i>RDSH</i>
C_6H_5^+	18.72	?	PI	Jochims, Rasekh, et al., 1993	<i>LL</i>
C_6H_5^+	18.6 ± 0.1	$\text{C}_2\text{H}_2 + \text{C}_2\text{H}$	PI	Jochims, Rasekh, et al., 1992	<i>LL</i>
C_6H_5^+	18.45 ± 0.05	?	EI	VanBrunt and Wacks, 1964	<i>RDSH</i>
C_6H_6^+	15.64	C_4H_2	PI	Jochims, Rasekh, et al., 1993	<i>LL</i>
C_6H_6^+	15.7 ± 0.1	C_4H_2	PI	Jochims, Rasekh, et al., 1992	<i>LL</i>
C_6H_6^+	15.20 ± 0.05	?	EI	VanBrunt and Wacks, 1964	<i>RDSH</i>
C_7H_3^+	20.66 ± 0.15	$\text{C}_3\text{H}_3 + \text{H}_2$	PI	Jochims, Rasekh, et al., 1992	<i>LL</i>
C_7H_5^+	15.90	C_3H_3	PI	Jochims, Rasekh, et al., 1993	<i>LL</i>
C_7H_5^+	16.1 ± 0.1	C_3H_3	PI	Jochims, Rasekh, et al., 1992	<i>LL</i>
C_8H_5^+	19.00 ± 0.05	$\text{C}_2\text{H}_2 + \text{H}$	PI	Jochims, Rasekh, et al., 1992	<i>LL</i>
C_8H_5^+	18.07 ± 0.05	?	EI	VanBrunt and Wacks, 1964	<i>RDSH</i>
C_8H_6^+	15.50	C_2H_2	PI	Jochims, Rasekh, et al., 1993	<i>LL</i>
C_8H_6^+	12.74	C_2H_2	EVAL	Gotkis, Oleinikova, et al., 1993	T = 0K; <i>LL</i>
C_8H_6^+	14.43	C_2H_2	TRPI	Gotkis, Oleinikova, et al., 1993	<i>LL</i>
C_8H_6^+	15.4 ± 0.1	C_2H_2	PI	Jochims, Rasekh, et al., 1992	<i>LL</i>
C_8H_6^+	15.4 ± 0.10	C_2H_2	EI	VanBrunt and Wacks, 1964	<i>RDSH</i>

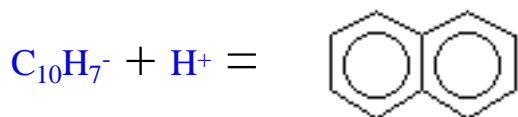
$C_{10}H_6^+$	15.60 ± 0.05	H_2	PI	Jochims, Rasekh, et al., 1992	<i>LL</i>
$C_{10}H_6^+$	16.2 ± 0.15	H_2	EI	VanBrunt and Wacks, 1964	<i>RDSH</i>
$C_{10}H_7^+$	15.41	H	PI	Jochims, Rasekh, et al., 1993	<i>LL</i>
$C_{10}H_7^+$	12.37	H	EVAL	Gotkis, Oleinikova, et al., 1993	T = 0K; <i>LL</i>
$C_{10}H_7^+$	14.24	H	TRPI	Gotkis, Oleinikova, et al., 1993	<i>LL</i>
$C_{10}H_7^+$	15.4 ± 0.1	H	PI	Jochims, Rasekh, et al., 1992	<i>LL</i>
$C_{10}H_7^+$	15.4 ± 0.10	H	EI	VanBrunt and Wacks, 1964	<i>RDSH</i>

De-protonation reactions



By formula: $C_{10}H_7^- + H^+ = C_{10}H_8$

Quantity	Value	Units	Method	Reference	Comment
$\Delta_r H^\circ$	$1649. \pm 5.0$	kJ/mol	Bran	Reed and Kass, 2000	gas phase; <i>B</i>
$\Delta_r H^\circ$	$1649. \pm 5.0$	kJ/mol	TDEq	Meot-ner, Liebman, et al., 1988	gas phase; Pyridazine. Anchored to Meot-ner, 1988 scale, not the "87 Acidity Scale".; <i>B</i>
$\Delta_r H^\circ$	$1648. \pm 21.$	kJ/mol	CIDC	Lardin, Squires, et al., 2001	gas phase; <i>B</i>
Quantity	Value	Units	Method	Reference	Comment
$\Delta_r G^\circ$	$1613. \pm 5.4$	kJ/mol	H-TS	Reed and Kass, 2000	gas phase; <i>B</i>
$\Delta_r G^\circ$	$1606. \pm 5.0$	kJ/mol	TDEq	Meot-ner, Liebman, et al., 1988	gas phase; Pyridazine. Anchored to Meot-ner, 1988 scale, not the "87 Acidity Scale".; <i>B</i>
$\Delta_r G^\circ$	$1613. \pm 21.$	kJ/mol	H-TS	Lardin, Squires, et al., 2001	gas phase; <i>B</i>



By formula: $\text{C}_{10}\text{H}_7^- + \text{H}^+ = \text{C}_{10}\text{H}_8$

Quantity	Value	Units	Method	Reference	Comment
$\Delta_f H^\circ$	$1655. \pm 5.4$	kJ/mol	Bran	Reed and Kass, 2000	gas phase; <i>B</i>
Quantity	Value	Units	Method	Reference	Comment
$\Delta_f G^\circ$	$1619. \pm 5.9$	kJ/mol	H-TS	Reed and Kass, 2000	gas phase; <i>B</i>

References

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