Naphthacene

Other names:	2,3-Benzanthracene
	2,3-Benzanthrene
	Benz[b]anthracene
	Benzo[b]anthracene
	CHRYSOGEN
	METHACENE
	Napthacene
	RUBENE
	Tetracen
	Tetracene
	Tetracene (hydrocarbon)
Inchi:	InChI=1S/C18H12/c1-2-6-14-10-18-12-16-8-4-3-7-15(16)11-17(18)9-13(14)5-1/h1-12H
InchiKey:	IFLREYGFSNHWGE-UHFFFAOYSA-N
Formula:	C18H12
SMILES:	c1ccc2cc3cc4ccccc4cc3cc2c1
Mol. weight [g/mol]:	228.29
CAS:	92-24-0

Physical Properties

Property code	Value	Unit	Source
affp	908.30	kJ/mol	NIST Webbook
affp	905.50	kJ/mol	NIST Webbook
basg	876.50	kJ/mol	NIST Webbook
basg	884.10	kJ/mol	NIST Webbook
chs	-8956.90 ± 1.30	kJ/mol	NIST Webbook
ea	1.06 ± 0.01	eV	NIST Webbook
ea	0.88 ± 0.04	eV	NIST Webbook
ea	1.07 ± 0.04	eV	NIST Webbook
gf	513.78	kJ/mol	Joback Method
hf	342.60 ± 5.90	kJ/mol	NIST Webbook
hfs	206.70 ± 3.00	kJ/mol	NIST Webbook
hfus	36.80	kJ/mol	Heat Capacities of Tetracene and Pentacene
hsub	143.70 ± 0.50	kJ/mol	NIST Webbook
hsub	125.00	kJ/mol	NIST Webbook
hsub	136.10 ± 0.30	kJ/mol	NIST Webbook
hsub	144.00 ± 5.00	kJ/mol	NIST Webbook

hvap	106.20 ± 3.70	kJ/mol	NIST Webbook
ie	7.00 ± 0.30	eV	NIST Webbook
ie	7.01	eV	NIST Webbook
ie	6.97 ± 0.02	eV	NIST Webbook
ie	6.64	eV	NIST Webbook
ie	7.00	eV	NIST Webbook
ie	7.00	eV	NIST Webbook
ie	6.90	eV	NIST Webbook
ie	6.95	eV	NIST Webbook
ie	6.94	eV	NIST Webbook
ie	7.01	eV	NIST Webbook
ie	7.04 ± 0.04	eV	NIST Webbook
ie	7.04	eV	NIST Webbook
ie	6.97	eV	NIST Webbook
ie	6.90 ± 0.30	eV	NIST Webbook
ie	6.97	eV	NIST Webbook
ie	6.97 ± 0.05	eV	NIST Webbook
log10ws	-8.60		Aqueous Solubility Prediction Method
log10ws	-8.60		Estimated Solubility Method
logp	5.146		Crippen Method
mcvol	182.340	ml/mol	McGowan Method
pc	2511.00	kPa	KDB
rinpol	2425.00		NIST Webbook
rinpol	2425.00		NIST Webbook
rinpol	2386.00		NIST Webbook
rinpol	2436.00		NIST Webbook
rinpol	2395.00		NIST Webbook
rinpol	405.00		NIST Webbook
rinpol	403.50		NIST Webbook
rinpol	403.15		NIST Webbook
rinpol	2426.00		NIST Webbook
rinpol	407.30		NIST Webbook
rinpol	403.52		NIST Webbook
rinpol	408.30		NIST Webbook
rinpol	401.28		NIST Webbook
rinpol	405.70		NIST Webbook
rinpol	403.51		NIST Webbook
rinpol	403.70		NIST Webbook
rinpol	403.89		NIST Webbook
rinpol	408.30		NIST Webbook
rinpol	2395.00		NIST Webbook
rinpol	402.86		NIST Webbook
rinpol	403.90		NIST Webbook

ss	215.40	J/mol×K	NIST Webbook
tb	704.82	K	Joback Method
tc	987.20	K	KDB
tf	613.15 ± 2.00	K	NIST Webbook
tf	625.55	K	Aqueous Solubility Prediction Method
tf	608.00	K	KDB
tf	613.15 ± 2.00	K	NIST Webbook
tt	623.75	K	Solubilities of Organic Semiconductors and Nonsteroidal Anti-inflammatory Drugs in Pure and Mixed Organic Solvents: Measurement and Modeling with Hansen Solubility Parameter
vc	0.700	m3/kmol	KDB
zc	0.2141430		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.24	J/mol×K	968.39	Joback Method
cpg	482.86	J/mol×K	748.75	Joback Method
cpg	496.51	J/mol×K	792.68	Joback Method
cpg	509.15	J/mol×K	836.61	Joback Method
cpg	521.02	J/mol×K	880.54	Joback Method
cpg	532.31	J/mol×K	924.47	Joback Method
cpg	468.00	J/mol×K	704.82	Joback Method
cps	236.60	J/mol×K	298.15	NIST Webbook
dvisc	0.0007153	Pa×s	704.82	Joback Method
dvisc	0.0010040	Pa×s	573.50	Joback Method
dvisc	0.0011669	Pa×s	529.73	Joback Method
dvisc	0.0007890	Pa×s	661.05	Joback Method
dvisc	0.0013935	Pa×s	485.95	Joback Method
dvisc	0.0017235	Pa×s	442.18	Joback Method
dvisc	0.0008825	Pa×s	617.27	Joback Method
hsubt	117.20	kJ/mol	459.00	NIST Webbook
hsubt	132.60	kJ/mol	458.00	NIST Webbook
hsubt	128.80	kJ/mol	463.00	NIST Webbook
hsubt	125.00 ± 4.00	kJ/mol	422.00	NIST Webbook
hsubt	126.50	kJ/mol	383.00	NIST Webbook
hsubt	126.10 ± 9.00	kJ/mol	429.00	NIST Webbook
hsubt	124.80 ± 2.60	kJ/mol	414.50	NIST Webbook

hsubt	124.00	kJ/mol	293.00	NIST Webbook
psub	5.42e-05	kPa	414.60	Sublimation Thermodynamic Parameters for Cholesterol, Ergosterol,
psub	7.84e-05	kPa	418.60	Sublimation Thermodynamic Parameters for Cholesterol, Ergosterol,
psub	8.46e-05	kPa	419.60	Sublimation Thermodynamic Parameters for Cholesterol, Ergosterol,
psub	1.03e-04	kPa	420.80	Sublimation Thermodynamic Parameters for Cholesterol, Ergosterol,
psub	1.28e-04	kPa	424.70	Sublimation Thermodynamic Parameters for Cholesterol, Ergosterol,
psub	2.15e-04	kPa	430.10	Sublimation Thermodynamic Parameters for Cholesterol, Ergosterol,
psub	6.39e-05	kPa	416.60	Sublimation Thermodynamic Parameters for Cholesterol, Ergosterol,
psub	6.67e-05	kPa	415.80	Sublimation Thermodynamic Parameters for Cholesterol, Ergosterol,
psub	4.22e-05	kPa	410.60	Sublimation Thermodynamic Parameters for Cholesterol, Ergosterol,
psub	3.39e-05	kPa	409.50	Sublimation Thermodynamic Parameters for Cholesterol, Ergosterol,
psub	2.10e-05	kPa	404.40	Sublimation Thermodynamic Parameters for Cholesterol, Ergosterol,
psub	1.46e-05	kPa	399.00	Sublimation Thermodynamic Parameters for Cholesterol, Ergosterol,

psub	2.55e-05	kPa	405.60	Sublimation Thermodynamic Parameters for Cholesterol, Ergosterol,
pvap	1.24e-07	kPa	298.15	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.72e-04	kPa	370.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	8.40e-04	kPa	380.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.80e-03	kPa	390.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.66e-03	kPa	400.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	7.11e-03	kPa	410.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	0.01	kPa	420.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.02	kPa	430.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.04	kPa	440.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.07	kPa	450.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.11	kPa	460.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.18	kPa	470.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.27	kPa	480.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	0.40	kPa	490.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.59	kPa	500.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.55e-04	kPa	360.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.05e-05	kPa	350.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.20e-05	kPa	340.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	7.39e-06	kPa	330.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.28e-06	kPa	320.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	6.39e-07	kPa	310.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.62e-07	kPa	300.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.85	kPa	510.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.74648e+01
Coeff. B	-1.54566e+04
Coeff. C	3.15863e-03
Coeff. D	-2.56685e-09
Temperature range (K), min.	420.15
Temperature range (K), max.	449.15

Sources

Sublimation Thermodynamic Parameters for Cholesterol, Ergosterol,	https://www.doi.org/10.1021/je800395m
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solubilities of Organic Semiconductors and Nonsteroidal Anti-inflammatory Drugs in Pure and Mixed Organic Solvents: Measurement and Modeling with Hansen Solubility Parameter:	https://www.doi.org/10.1021/acs.jced.8b00536
Heat Capacities of Tetracene and Pentacene:	https://www.doi.org/10.1021/je800382b

Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons:	https://www.doi.org/10.1021/je800300x
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/files/research/kdb/mol/mol805.mol
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92240&Units=SI
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=805

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility