Benz[a]anthracene

Other names:	1,2-Benz[a]anthracene
	1,2-Benzanthracene
	1,2-Benzanthrazen
	1,2-Benzanthrene
	1,2-Benzoanthracene
	2,3-Benzophenanthrene
	2,3-Benzphenanthrene
	BA
	BENZANTHRENE
	BENZOANTHRACENE
	Benzanthracene
	Benzo[a]anthracene
	Benzo[b]phenanthrene
	NSC 30970
	Rcra waste number U018
	TETRAPHENE
Inchi:	InChI=1S/C18H12/c1-2-7-15-12-18-16(11-14(15)6-1)10-9-13-5-3-4-8-17(13)18/h1-12H
InchiKey:	DXBHBZVCASKNBY-UHFFFAOYSA-N
Formula:	C18H12
SMILES:	c1ccc2cc3c(ccc4ccccc43)cc2c1
Mol. weight [g/mol]:	228.29
CAS:	56-55-3

Physical Properties

Property code	Value	Unit	Source
chs	-8969.00 ± 2.30	kJ/mol	NIST Webbook
ea	0.63 ± 0.01	eV	NIST Webbook
ea	0.39 ± 0.10	eV	NIST Webbook
ea	0.46	eV	NIST Webbook
gf	513.78	kJ/mol	Joback Method
hf	290.30 ± 6.00	kJ/mol	NIST Webbook
hfs	170.80 ± 3.30	kJ/mol	NIST Webbook
hfus	26.70	kJ/mol	Joback Method
hsub	119.50 ± 5.00	kJ/mol	NIST Webbook
hsub	123.00 ± 3.00	kJ/mol	NIST Webbook
hsub	120.00	kJ/mol	NIST Webbook
hsub	123.00 ± 3.00	kJ/mol	NIST Webbook

hvap	105.80 ± 1.90	kJ/mol	NIST Webbook
hvap	96.60 ± 1.40	kJ/mol	NIST Webbook
ie	7.60	eV	NIST Webbook
ie	7.50	eV	NIST Webbook
ie	7.47 ± 0.01	eV	NIST Webbook
ie	7.35	eV	NIST Webbook
ie	7.56 ± 0.01	eV	NIST Webbook
ie	7.53	eV	NIST Webbook
ie	7.45	eV	NIST Webbook
ie	7.50 ± 0.30	eV	NIST Webbook
ie	7.45 ± 0.05	eV	NIST Webbook
ie	7.42	eV	NIST Webbook
ie	7.46 ± 0.03	eV	NIST Webbook
ie	7.41 ± 0.02	eV	NIST Webbook
ie	7.56	eV	NIST Webbook
ie	7.52	eV	NIST Webbook
ie	7.41	eV	NIST Webbook
log10ws	-7.21		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	5.146		Crippen Method
mcvol	182.340	ml/mol	McGowan Method
pc	2511.00	kPa	KDB
rinpol	398.33		NIST Webbook
rinpol	2447.00		NIST Webbook
rinpol	2452.00		NIST Webbook
rinpol	2447.00		NIST Webbook
rinpol	2418.00		NIST Webbook
rinpol	2421.00		NIST Webbook
rinpol	2445.00		NIST Webbook
rinpol	2403.00		NIST Webbook
rinpol	398.96		NIST Webbook
rinpol	401.97		NIST Webbook
rinpol	399.22		NIST Webbook
rinpol	399.00		NIST Webbook
rinpol	399.71		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	398.20		NIST Webbook
rinpol	398.50		NIST Webbook
rinpol	398.60		NIST Webbook
rinpol	398.60		NIST Webbook
rinpol	398.69		NIST Webbook
rinpol	398.51		NIST Webbook
rinpol	398.53		NIST Webbook
rinpol	398.57		NIST Webbook

rinpol	398.26	NIST Webbook
rinpol	398.55	NIST Webbook
rinpol	398.59	NIST Webbook
rinpol	398.60	NIST Webbook
rinpol	398.62	NIST Webbook
rinpol	398.63	NIST Webbook
rinpol	398.64	NIST Webbook
rinpol	398.64	NIST Webbook
rinpol	398.63	NIST Webbook
rinpol	398.72	NIST Webbook
rinpol	2441.00	NIST Webbook
rinpol	398.36	NIST Webbook
rinpol	398.10	NIST Webbook
rinpol	398.50	NIST Webbook
rinpol	398.22	NIST Webbook
rinpol	398.14	NIST Webbook
rinpol	398.40	NIST Webbook
rinpol	398.69	NIST Webbook
rinpol	398.50	NIST Webbook
rinpol	398.77	NIST Webbook
rinpol	2440.00	NIST Webbook
rinpol	397.55	NIST Webbook
rinpol	398.76	NIST Webbook
rinpol	398.50	NIST Webbook
rinpol	398.20	NIST Webbook
rinpol	398.36	NIST Webbook
rinpol	398.36	NIST Webbook
rinpol	398.69	NIST Webbook
rinpol	398.76	NIST Webbook
rinpol	398.40	NIST Webbook
rinpol	397.70	NIST Webbook
rinpol	398.31	NIST Webbook
rinpol	398.40	NIST Webbook
rinpol	398.30	NIST Webbook
rinpol	398.40	NIST Webbook
rinpol	398.60	NIST Webbook
rinpol	398.70	NIST Webbook
rinpol	398.60	NIST Webbook
rinpol	398.36	NIST Webbook
rinpol	398.40	NIST Webbook
rinpol	398.70	NIST Webbook
rinpol	400.29	NIST Webbook
rinpol	398.50	NIST Webbook
rinpol	398.76	NIST Webbook

rinpol	396.46		NIST Webbook
rinpol	398.41		NIST Webbook
rinpol	398.50		NIST Webbook
rinpol	399.10		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	396.38		NIST Webbook
rinpol	394.44		NIST Webbook
rinpol	396.70		NIST Webbook
rinpol	397.95		NIST Webbook
rinpol	398.46		NIST Webbook
rinpol	398.47		NIST Webbook
rinpol	398.50		NIST Webbook
rinpol	398.59		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	2440.00		NIST Webbook
rinpol	2393.00		NIST Webbook
rinpol	398.20		NIST Webbook
rinpol	398.51		NIST Webbook
rinpol	398.59		NIST Webbook
rinpol	398.64		NIST Webbook
rinpol	398.10		NIST Webbook
rinpol	398.69		NIST Webbook
rinpol	398.76		NIST Webbook
rinpol	2403.00		NIST Webbook
rinpol	2423.00		NIST Webbook
rinpol	2403.00		NIST Webbook
rinpol	2389.00		NIST Webbook
rinpol	2400.00		NIST Webbook
rinpol	2432.80		NIST Webbook
rinpol	2433.59		NIST Webbook
rinpol	2453.00		NIST Webbook
rinpol	2453.00		NIST Webbook
rinpol	398.60		NIST Webbook
tb	710.80	K	NIST Webbook
tb	710.70 ± 2.00	K	NIST Webbook
tb	710.80 ± 2.00	K	NIST Webbook
tb	710.70 ± 2.00	K	NIST Webbook
tb	710.80 ± 2.00	K	NIST Webbook
tb	708.00	K	KDB
tc	998.20	K	KDB
tf	433.70 ± 1.40	K	NIST Webbook
tf	434.00 ± 2.00	K	NIST Webbook
tf	430.40 ± 1.00	K	NIST Webbook
tf	434.40 ± 0.60	K	NIST Webbook

tf	432.00 ± 3.00	K	NIST Webbook
tf	434.30 ± 0.40	K	NIST Webbook
tf	430.10 ± 2.00	K	NIST Webbook
tf	431.00 ± 2.00	K	NIST Webbook
tf	428.00	K	KDB
vc	0.700	m3/kmol	KDB
zc	0.2117830		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.51	J/mol×K	792.68	Joback Method
cpg	468.00	J/mol×K	704.82	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	543.24	J/mol×K	968.39	Joback Method
cpg	482.86	J/mol×K	748.75	Joback Method
cps	273.60	J/mol×K	298.15	NIST Webbook
dvisc	0.0008825	Pa×s	617.27	Joback Method
dvisc	0.0007153	Pa×s	704.82	Joback Method
dvisc	0.0017235	Pa×s	442.18	Joback Method
dvisc	0.0013935	Pa×s	485.95	Joback Method
dvisc	0.0011669	Pa×s	529.73	Joback Method
dvisc	0.0010040	Pa×s	573.50	Joback Method
dvisc	0.0007890	Pa×s	661.05	Joback Method
hfust	20.10	kJ/mol	433.50	NIST Webbook
hfust	21.38	kJ/mol	434.30	NIST Webbook
hfust	21.38	kJ/mol	434.30	NIST Webbook
hsubt	113.40	kJ/mol	360.00	NIST Webbook
hsubt	109.00	kJ/mol	293.00	NIST Webbook
hsubt	120.50	kJ/mol	405.50	NIST Webbook
hsubt	104.60	kJ/mol	377.00	NIST Webbook
hsubt	104.60 ± 4.20	kJ/mol	390.00	NIST Webbook
hsubt	119.70	kJ/mol	363.00	NIST Webbook
hsubt	117.00	kJ/mol	333.00	NIST Webbook
hsubt	115.50	kJ/mol	383.00	NIST Webbook
hsubt	104.00 ± 2.00	kJ/mol	351.00	NIST Webbook
hvapt	91.00	kJ/mol	398.00	NIST Webbook

pvap	0.95	kPa	510.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.45	kPa	490.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.30	kPa	480.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.20	kPa	470.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.13	kPa	460.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.08	kPa	450.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.05	kPa	440.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	0.03	kPa	430.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.02	kPa	420.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	8.33e-03	kPa	410.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.31e-03	kPa	400.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.13e-03	kPa	390.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.00e-03	kPa	380.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.46e-04	kPa	370.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	1.87e-04	kPa	360.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	7.35e-05	kPa	350.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.66	kPa	500.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	9.10e-06	kPa	330.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.83e-06	kPa	320.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	7.97e-07	kPa	310.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.03e-07	kPa	300.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	1.56e-07	kPa	298.15	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.69e-05	kPa	340.00	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	1.27171e+01
Coeff. B	-1.29437e+04
Coeff. C	2.21615e+00
Coeff. D	-1.25878e-06
Temperature range (K), min.	371.15
Temperature range (K), max.	395.15

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Determination of Henry's Law Constant Using Diffusion in Air and Water Boundary Layers:	https://www.doi.org/10.1021/je300954s
KDB:	https://www.cheric.org/files/research/kdb/mol/mol804.mol
Solubility of Solid Polycyclic Aromatic Hydrocarbons in Pressurized Hot Water at Temperatures from 313 K to the Melting Point:	https://www.doi.org/10.1021/je050427r
Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons:	https://www.doi.org/10.1021/je800300x
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56553&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=804

Legend

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility