Benzo[a]pyrene

Other names:	1,2-Benzpyrene
	3,4-BP
	3,4-Benz[a]pyrene
	3,4-Benzopirene
	3,4-Benzopyrene
	3,4-Benzpyren
	3,4-Benzpyrene
	4,5-Benzpyrene
	6,7-Benzopyrene
	B(a)P
	BP
	Benz[a]pyrene
	Benzo(a)pyrene
	Benzo[d,e,f]chrysene
	Benzo[«alpha»]pyrene
	Benzo[Â«alphaÂ»]pyrene
	Benzopyrene
	NSC 21914
	Rcra waste number U022
	benzo(d,e,f)chrysene
Inchi:	InChI=1S/C20H12/c1-2-7-17-15(4-1)12-16-9-8-13-5-3-6-14-10-11-18(17)20(16)19(13)14/
InchiKey:	FMMWHPNWAFZXNH-UHFFFAOYSA-N
Formula:	C20H12
SMILES:	c1ccc2c(c1)cc1ccc3cccc4ccc2c1c34
Mol. weight [g/mol]:	252.31
CAS:	50-32-8

Physical Properties

Property code	Value	Unit	Source
ea	0.68 ± 0.01	eV	NIST Webbook
ea	0.81 ± 0.04	eV	NIST Webbook
gf	621.88	kJ/mol	Joback Method
hf	464.81	kJ/mol	Joback Method
hfus	31.48	kJ/mol	Joback Method
hvap	117.80 ± 1.00	kJ/mol	NIST Webbook
hvap	105.00 ± 1.50	kJ/mol	NIST Webbook
ie	7.60	eV	NIST Webbook

ie	7.10	eV	NIST Webbook
ie	7.41	eV	NIST Webbook
ie	7.12	eV	NIST Webbook
ie	7.12 ± 0.01	eV	NIST Webbook
ie	7.73	eV	NIST Webbook
ie	7.56	eV	NIST Webbook
ie	7.12 ± 0.01	eV	NIST Webbook
ie	7.39 ± 0.01	eV	NIST Webbook
log10ws	-8.70		Estimated Solubility Method
log10ws	-8.03		Aqueous Solubility Prediction Method
log10ws	-7.82		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	5.737		Crippen Method
mcvol	195.360	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	2778.00		NIST Webbook
rinpol	2769.00		NIST Webbook
rinpol	2790.00		NIST Webbook
rinpol	2790.00		NIST Webbook
rinpol	2790.00		NIST Webbook
rinpol	2790.00		NIST Webbook
rinpol	2800.00		NIST Webbook
rinpol	2800.00		NIST Webbook
rinpol	2800.00		NIST Webbook
rinpol	2812.00		NIST Webbook
rinpol	2823.00		NIST Webbook
rinpol	2824.00		NIST Webbook
rinpol	2773.00		NIST Webbook
rinpol	2760.00		NIST Webbook
rinpol	2798.00		NIST Webbook
rinpol	2838.00		NIST Webbook
rinpol	2839.00		NIST Webbook
rinpol	2849.00		NIST Webbook
rinpol	2849.00		NIST Webbook
rinpol	2830.00		NIST Webbook
rinpol	453.40		NIST Webbook
rinpol	454.70		NIST Webbook
rinpol	453.90		NIST Webbook
rinpol	455.40		NIST Webbook
rinpol	453.70		NIST Webbook
rinpol	453.44		NIST Webbook
rinpol	453.40		NIST Webbook

rinpol	454.87	NIST Webbook
rinpol	454.57	NIST Webbook
rinpol	454.06	NIST Webbook
rinpol	451.88	NIST Webbook
rinpol	446.90	NIST Webbook
rinpol	446.94	NIST Webbook
rinpol	447.00	NIST Webbook
rinpol	447.05	NIST Webbook
rinpol	447.06	NIST Webbook
rinpol	447.13	NIST Webbook
rinpol	447.44	NIST Webbook
rinpol	447.45	NIST Webbook
rinpol	452.99	NIST Webbook
rinpol	453.05	NIST Webbook
rinpol	454.18	NIST Webbook
rinpol	454.02	NIST Webbook
rinpol	455.41	NIST Webbook
rinpol	440.30	NIST Webbook
rinpol	455.80	NIST Webbook
rinpol	451.00	NIST Webbook
rinpol	454.50	NIST Webbook
rinpol	456.40	NIST Webbook
rinpol	454.30	NIST Webbook
rinpol	452.30	NIST Webbook
rinpol	2769.00	NIST Webbook
rinpol	453.62	NIST Webbook
rinpol	453.36	NIST Webbook
rinpol	454.57	NIST Webbook
rinpol	448.69	NIST Webbook
rinpol	453.40	NIST Webbook
rinpol	454.42	NIST Webbook
rinpol	451.20	NIST Webbook
rinpol	454.02	NIST Webbook
rinpol	453.44	NIST Webbook
rinpol	440.70	NIST Webbook
rinpol	455.14	NIST Webbook
rinpol	454.02	NIST Webbook
rinpol	454.57	NIST Webbook
rinpol	455.14	NIST Webbook
rinpol	454.30	NIST Webbook
rinpol	446.20	NIST Webbook
rinpol	451.34	NIST Webbook
rinpol	451.59	NIST Webbook
rinpol	453.40	NIST Webbook

rinpol	453.40		NIST Webbook
rinpol	453.40		NIST Webbook
rinpol	453.40		NIST Webbook
rinpol	451.59		NIST Webbook
rinpol	451.92		NIST Webbook
rinpol	454.75		NIST Webbook
rinpol	455.33		NIST Webbook
rinpol	453.44		NIST Webbook
rinpol	454.02		NIST Webbook
rinpol	453.74		NIST Webbook
rinpol	454.38		NIST Webbook
rinpol	452.95		NIST Webbook
rinpol	454.33		NIST Webbook
rinpol	451.80		NIST Webbook
rinpol	453.22		NIST Webbook
rinpol	441.53		NIST Webbook
rinpol	451.08		NIST Webbook
rinpol	2769.00		NIST Webbook
rinpol	452.56		NIST Webbook
rinpol	453.05		NIST Webbook
rinpol	453.15		NIST Webbook
rinpol	453.44		NIST Webbook
rinpol	454.41		NIST Webbook
rinpol	453.40		NIST Webbook
rinpol	2838.00		NIST Webbook
rinpol	2769.00		NIST Webbook
rinpol	2766.00		NIST Webbook
rinpol	2809.20		NIST Webbook
rinpol	2828.00		NIST Webbook
rinpol	2822.00		NIST Webbook
rinpol	2828.00		NIST Webbook
rinpol	2817.00		NIST Webbook
rinpol	2813.00		NIST Webbook
rinpol	2809.00		NIST Webbook
rinpol	2778.00		NIST Webbook
rinpol	2764.00		NIST Webbook
rinpol	2763.00		NIST Webbook
rinpol	454.55		NIST Webbook
rinpol	452.46		NIST Webbook
tb	768.20	K	NIST Webbook
tc	1030.60	K	Joback Method
tf	450.00 ± 3.00	K	NIST Webbook
tf	450.20 ± 2.00	K	NIST Webbook
tf	452.40 ± 1.50	K	NIST Webbook

tf	449.00 ± 3.00	K	NIST Webbook
tf	449.60 ± 2.00	K	NIST Webbook
tf	450.00	K	NIST Webbook
tf	451.00 ± 2.00	K	NIST Webbook
tf	450.77	K	Aqueous Solubility Prediction Method
tf	449.20 ± 2.00	K	NIST Webbook
tf	447.00 ± 5.00	K	NIST Webbook
tf	454.00 ± 2.00	K	NIST Webbook
tf	453.00 ± 1.00	K	NIST Webbook
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	584.31	J/mol×K	986.64	Joback Method
cpg	559.83	J/mol×K	898.72	Joback Method
cpg	547.49	J/mol×K	854.76	Joback Method
cpg	534.69	J/mol×K	810.80	Joback Method
cpg	521.16	J/mol×K	766.84	Joback Method
cpg	597.00	J/mol×K	1030.60	Joback Method
cpg	572.01	J/mol×K	942.68	Joback Method
dvisc	0.0029976	Pa×s	557.99	Joback Method
dvisc	0.0027980	Pa×s	599.76	Joback Method
dvisc	0.0026352	Pa×s	641.53	Joback Method
dvisc	0.0025002	Pa×s	683.30	Joback Method
dvisc	0.0023865	Pa×s	725.07	Joback Method
dvisc	0.0032474	Pa×s	516.22	Joback Method
dvisc	0.0022895	Pa×s	766.84	Joback Method
hfust	17.32	kJ/mol	454.20	NIST Webbook
hfust	14.70	kJ/mol	451.80	NIST Webbook
hfust	17.32	kJ/mol	454.20	NIST Webbook
hfust	8.49	kJ/mol	390.20	NIST Webbook
hsubt	118.30	kJ/mol	394.50	NIST Webbook
hsubt	122.50	kJ/mol	383.00	NIST Webbook
hvapt	95.50	kJ/mol	398.00	NIST Webbook
hvapt	91.00	kJ/mol	398.00	NIST Webbook

psub	1.02e-03	kPa	423.90	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	7.96e-05	kPa	393.50	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	1.29e-04	kPa	397.80	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	1.67e-04	kPa	400.80	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	1.80e-04	kPa	402.30	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	2.17e-04	kPa	405.20	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	2.73e-04	kPa	406.60	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method

psub	3.94e-04	kPa	411.50	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	4.18e-04	kPa	411.80	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	7.31e-05	kPa	392.30	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	5.37e-04	kPa	415.50	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	6.97e-04	kPa	419.00	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	7.33e-04	kPa	419.70	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	7.85e-04	kPa	421.20	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	

psub	9.80e-04	kPa	423.80	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	4.94e-04	kPa	415.10	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
pvap	6.95e-09	kPa	298.15	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	9.35e-09	kPa	300.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.31e-08	kPa	310.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.77e-07	kPa	320.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.56e-07	kPa	330.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	2.20e-06	kPa	340.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.78e-06	kPa	350.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.93e-05	kPa	360.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	5.09e-05	kPa	370.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.26e-04	kPa	380.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.26	kPa	510.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.41e-04	kPa	400.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	1.34e-03	kPa	410.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.66e-03	kPa	420.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	5.06e-03	kPa	430.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	9.25e-03	kPa	440.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.02	kPa	450.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.03	kPa	460.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.05	kPa	470.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	0.07	kPa	480.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.11	kPa	490.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.17	kPa	500.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.92e-04	kPa	390.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
sfust	38.13	J/mol×K	454.20	NIST Webbook
sfust	21.77	J/mol×K	390.20	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	584.00 ± 1.00	K	1.30	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method:	https://www.doi.org/10.1021/je7005133
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50328&Units=SI
Determination of Henry's Law Constant Using Diffusion in Air and Water Boundary Layers:	https://www.doi.org/10.1021/je300954s
Hypothetical Thermodynamic Properties. Subcooled Vaporization Estimated Solubility Method:	https://www.doi.org/10.1021/je800300x
Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
psub:	Sublimation pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume