Benzo[e]pyrene

Other names:	1,2-benzopyrene
	192-97-2
	4,5-Benzopyrene
	4,5-Benzpyrene
	9,10-Benzpyrene
	B(e)P
	Benz(e)pyrene
	Benzo(e)pyrene
	Benzo(l)pyrene
Inchi:	InChI=1S/C20H12/c1-2-8-16-15(7-1)17-9-3-5-13-11-12-14-6-4-10-18(16)20(14)19(13)17/
InchiKey:	TXVHTIQJNYSSKO-UHFFFAOYSA-N
Formula:	C20H12
SMILES:	c1ccc2c(c1)c1cccc3ccc4cccc2c4c31
Mol. weight [g/mol]:	252.31
CAS:	192-97-2

Physical Properties

Property code	Value	Unit	Source
ea	0.53 ± 0.01	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	105.00 ± 1.50	kJ/mol	NIST Webbook
hvap	118.20 ± 0.30	kJ/mol	NIST Webbook
ie	7.41	eV	NIST Webbook
ie	7.43 ± 0.04	eV	NIST Webbook
ie	7.19	eV	NIST Webbook
ie	7.15	eV	NIST Webbook
ie	7.37	eV	NIST Webbook
log10ws	-7.80		Estimated Solubility Method
log10ws	-7.80		Aqueous Solubility Prediction Method
logp	5.737		Crippen Method
mcvol	195.360	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	2806.00		NIST Webbook

rinpol	450.73	NIST Webbook
rinpol	450.82	NIST Webbook
rinpol	2753.00	NIST Webbook
rinpol	2753.00	NIST Webbook
rinpol	2766.00	NIST Webbook
rinpol	2799.00	NIST Webbook
rinpol	2801.00	NIST Webbook
rinpol	450.75	NIST Webbook
rinpol	2817.00	NIST Webbook
rinpol	2816.00	NIST Webbook
rinpol	2816.00	NIST Webbook
rinpol	2794.40	NIST Webbook
rinpol	2770.65	NIST Webbook
rinpol	2751.03	NIST Webbook
rinpol	2817.50	NIST Webbook
rinpol	2816.00	NIST Webbook
rinpol	452.20	NIST Webbook
rinpol	452.60	NIST Webbook
rinpol	452.10	NIST Webbook
rinpol	453.30	NIST Webbook
rinpol	453.30	NIST Webbook
rinpol	450.73	NIST Webbook
rinpol	451.80	NIST Webbook
rinpol	453.12	NIST Webbook
rinpol	452.70	NIST Webbook
rinpol	452.22	NIST Webbook
rinpol	451.28	NIST Webbook
rinpol	452.36	NIST Webbook
rinpol	451.53	NIST Webbook
rinpol	454.10	NIST Webbook
rinpol	449.40	NIST Webbook
rinpol	452.40	NIST Webbook
rinpol	452.70	NIST Webbook
rinpol	453.10	NIST Webbook
rinpol	451.80	NIST Webbook
rinpol	452.86	NIST Webbook
rinpol	451.24	NIST Webbook
rinpol	452.70	NIST Webbook
rinpol	452.85	NIST Webbook
rinpol	449.80	NIST Webbook
rinpol	452.29	NIST Webbook
rinpol	450.73	NIST Webbook
rinpol	439.10	NIST Webbook
rinpol	452.93	NIST Webbook

rinpol	452.29		NIST Webbook
rinpol	452.70		NIST Webbook
rinpol	452.93		NIST Webbook
rinpol	452.70		NIST Webbook
rinpol	444.40		NIST Webbook
rinpol	449.38		NIST Webbook
rinpol	449.47		NIST Webbook
rinpol	450.70		NIST Webbook
rinpol	451.80		NIST Webbook
rinpol	452.70		NIST Webbook
rinpol	451.80		NIST Webbook
rinpol	450.10		NIST Webbook
rinpol	450.12		NIST Webbook
rinpol	452.86		NIST Webbook
rinpol	452.94		NIST Webbook
rinpol	450.73		NIST Webbook
rinpol	452.14		NIST Webbook
rinpol	452.71		NIST Webbook
rinpol	450.75		NIST Webbook
rinpol	452.65		NIST Webbook
rinpol	449.76		NIST Webbook
rinpol	450.73		NIST Webbook
rinpol	455.90		NIST Webbook
rinpol	450.73		NIST Webbook
rinpol	441.53		NIST Webbook
rinpol	449.62		NIST Webbook
rinpol	450.43		NIST Webbook
rinpol	450.73		NIST Webbook
rinpol	2794.40		NIST Webbook
rinpol	451.25		NIST Webbook
rinpol	452.23		NIST Webbook
rinpol	2817.50		NIST Webbook
rinpol	439.10		NIST Webbook
rinpol	452.70		NIST Webbook
rinpol	451.10		NIST Webbook
rinpol	452.86		NIST Webbook
rinpol	450.82		NIST Webbook
tb	766.84	K	Joback Method
tc	1030.60	K	Joback Method
tf	450.65	K	Aqueous Solubility Prediction Method
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	597.00	J/mol×K	1030.60	Joback Method
cpg	521.16	J/mol×K	766.84	Joback Method
cpg	534.69	J/mol×K	810.80	Joback Method
cpg	547.49	J/mol×K	854.76	Joback Method
cpg	559.83	J/mol×K	898.72	Joback Method
cpg	572.01	J/mol×K	942.68	Joback Method
dvisc	0.0023865	Pa×s	725.07	Joback Method
dvisc	0.0029976	Pa×s	557.99	Joback Method
dvisc	0.0032474	Pa×s	516.22	Joback Method
dvisc	0.0022895	Pa×s	766.84	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
hfust	2.51	kJ/mol	426.20	NIST Webbook
hfust	16.57	kJ/mol	454.40	NIST Webbook
hfust	13.80	kJ/mol	451.30	NIST Webbook
hfust	16.57	kJ/mol	454.40	NIST Webbook
hsubt	117.90	kJ/mol	383.00	NIST Webbook
hsubt	119.10	kJ/mol	391.00	NIST Webbook
hvapt	92.00	kJ/mol	398.00	NIST Webbook
pvap	6.94e-09	kPa	298.15	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.12	kPa	490.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	0.18	kPa	500.00	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	4.34e-08	kPa	310.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.79e-07	kPa	320.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.65e-07	kPa	330.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.24e-06	kPa	340.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.93e-06	kPa	350.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	1.97e-05	kPa	360.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	5.23e-05	kPa	370.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.30e-04	kPa	380.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.02e-04	kPa	390.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.64e-04	kPa	400.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.39e-03	kPa	410.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.76e-03	kPa	420.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	5.27e-03	kPa	430.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	9.65e-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	0.08	kPa	480.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.27	kPa	510.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

sfust	5.89	J/mol×K	426.20	NIST Webbook
sfust	36.46	J/mol×K	454.40	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	523.00	K	0.45	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C192972&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons:	https://www.doi.org/10.1021/je800300x

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

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