Benz[e]acephenanthrylene

Other names:	2,3-Benzofluoranthene
	2,3-Benzofluoranthrene
	2,3-benzfluoranthene
	205-99-2
	3,4-benz[e]acephenanthrylene
	3,4-benzfluoranthene
	3,4-benzofluoranthene
	4,5-Benzofluoranthene
	B(b)F
	Benz[b]fluoranthene
	Benzo(b)fluoranthene
	Benzo[e]acephenanthrylene
	NSC 89265
	benzo[b]fluoranthene
	benzo[e]fluoranthene
Inchi:	InChI=1S/C20H12/c1-2-7-14-13(6-1)12-19-16-9-4-3-8-15(16)18-11-5-10-17(14)20(18)19/
InchiKey:	FTOVXSOBNPWTSH-UHFFFAOYSA-N
Formula:	C20H12
SMILES:	c1ccc2c(c1)-c1cccc3c1c-2cc1ccccc13
Mol. weight [g/mol]:	252.32

Physical Properties

Property code	Value	Unit	Source
hf	360.35	kJ/mol	Cheméo Relay (1.0)
hfus	18.30	kJ/mol	Solid vapor pressure for five heavy PAHs via the Knudsen effusion method
hvap	116.80 ± 1.60	kJ/mol	NIST Webbook
hvap	104.00 ± 1.50	kJ/mol	NIST Webbook
ie	7.33	eV	Cheméo Relay (1.0)
log10ws	-8.23		Aqueous Solubility Prediction Method
log10ws	-8.23		Estimated Solubility Method
logp	5.640		Crippen Method
mcvol	195.360	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	448.07		NIST Webbook

rinpol	441.70	NIST Webbook
rinpol	2711.00	NIST Webbook
rinpol	2705.00	NIST Webbook
rinpol	443.90	NIST Webbook
rinpol	442.10	NIST Webbook
rinpol	442.60	NIST Webbook
rinpol	441.74	NIST Webbook
rinpol	442.10	NIST Webbook
rinpol	443.19	NIST Webbook
rinpol	443.11	NIST Webbook
rinpol	442.34	NIST Webbook
rinpol	440.81	NIST Webbook
rinpol	441.76	NIST Webbook
rinpol	441.80	NIST Webbook
rinpol	442.63	NIST Webbook
rinpol	443.65	NIST Webbook
rinpol	430.00	NIST Webbook
rinpol	444.00	NIST Webbook
rinpol	443.11	NIST Webbook
rinpol	439.51	NIST Webbook
rinpol	443.13	NIST Webbook
rinpol	441.74	NIST Webbook
rinpol	433.90	NIST Webbook
rinpol	448.07	NIST Webbook
rinpol	443.93	NIST Webbook
rinpol	2700.00	NIST Webbook
rinpol	443.11	NIST Webbook
rinpol	443.13	NIST Webbook
rinpol	443.93	NIST Webbook
rinpol	442.70	NIST Webbook
rinpol	435.40	NIST Webbook
rinpol	440.11	NIST Webbook
rinpol	2671.00	NIST Webbook
rinpol	442.10	NIST Webbook
rinpol	442.70	NIST Webbook
rinpol	442.10	NIST Webbook
rinpol	440.37	NIST Webbook
rinpol	440.37	NIST Webbook
rinpol	442.35	NIST Webbook
rinpol	443.58	NIST Webbook
rinpol	441.74	NIST Webbook
rinpol	443.13	NIST Webbook
rinpol	441.63	NIST Webbook
rinpol	460.35	NIST Webbook

rinpol	433.31		NIST Webbook
rinpol	433.31		NIST Webbook
rinpol	438.54		NIST Webbook
rinpol	439.41		NIST Webbook
rinpol	443.88		NIST Webbook
rinpol	441.74		NIST Webbook
rinpol	2671.00		NIST Webbook
rinpol	2705.00		NIST Webbook
rinpol	433.90		NIST Webbook
rinpol	443.13		NIST Webbook
rinpol	441.70		NIST Webbook
rinpol	440.37		NIST Webbook
rinpol	441.63		NIST Webbook
rinpol	439.41		NIST Webbook
rinpol	2700.00		NIST Webbook
rinpol	2694.00		NIST Webbook
tb	745.69	K	Cheméo Relay (1.0)
tc	1053.83	K	Cheméo Relay (1.0)
tf	448.91	K	Cheméo Relay (1.0)
vc	0.777	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	559.83	J/mol×K	898.72	Joback Method
cpg	584.31	J/mol×K	986.64	Joback Method
cpg	572.01	J/mol×K	942.68	Joback Method
cpg	597.00	J/mol×K	1030.60	Joback Method
dvisc	0.0022895	Pa×s	766.84	Joback Method
dvisc	0.0029976	Pa×s	557.99	Joback Method
dvisc	0.0023865	Pa×s	725.07	Joback Method
dvisc	0.0025002	Pa×s	683.30	Joback Method
dvisc	0.0026352	Pa×s	641.53	Joback Method
dvisc	0.0032474	Pa×s	516.22	Joback Method
dvisc	0.0027980	Pa×s	599.76	Joback Method
hfust	19.60	kJ/mol	441.50	NIST Webbook
hsubt	119.20	kJ/mol	383.00	NIST Webbook
hvapt	89.70	kJ/mol	398.00	NIST Webbook

pvap	2.60e-07	kPa	320.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.24	kPa	500.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.84e-03	kPa	410.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.64e-03	kPa	420.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.90e-03	kPa	430.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.01	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	0.04	kPa	460.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.06	kPa	470.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.10	kPa	480.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.15	kPa	490.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	8.84e-04	kPa	400.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.35	kPa	510.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.04e-04	kPa	390.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	1.75e-04	kPa	380.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	7.13e-05	kPa	370.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.72e-05	kPa	360.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	9.66e-06	kPa	350.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.17e-06	kPa	340.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	9.52e-07	kPa	330.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.40e-08	kPa	310.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	1.40e-08	kPa	300.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.05e-08	kPa	298.15	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

Sources

Solid vapor pressure for five heavy PAHs via the Knudsen effusion method:	https://www.doi.org/10.1016/j.jct.2011.05.030
Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons:	https://www.doi.org/10.1021/je800300x
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Ionic Liquids/Water Distribution Ratios of Some Polycyclic Aromatic Hydrocarbons:	https://www.doi.org/10.1021/je049879e
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=C205992&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume