Benzo[k]fluoranthene

Other names:	11,12-Benzofluoranthene
	2,3,1',8'-Binaphthylene
	8,9-Benzofluoranthene
	Benzo(k)fluoranthene
	Dibenzo[b,jk]fluorene
Inchi:	InChI=1S/C20H12/c1-2-6-15-12-19-17-10-4-8-13-7-3-9-16(20(13)17)18(19)11-14(15)5-1/
InchiKey:	HAXBIWFMXWRORI-UHFFFAOYSA-N
Formula:	C20H12
SMILES:	c1ccc2cc3c(cc2c1)-c1cccc2cccc-3c12
Mol. weight [g/mol]:	252.31
CAS:	207-08-9

Physical Properties

Property code	Value	Unit	Source
gf	621.88	kJ/mol	Joback Method
hf	306.20 ± 6.20	kJ/mol	NIST Webbook
hfs	172.40 ± 4.30	kJ/mol	NIST Webbook
hfus	26.50	kJ/mol	Solid vapor pressure for five heavy PAHs via the Knudsen effusion method
hsub	133.80 ± 4.50	kJ/mol	NIST Webbook
hsub	124.20 ± 4.70	kJ/mol	NIST Webbook
hvap	105.50 ± 1.50	kJ/mol	NIST Webbook
hvap	117.40 ± 1.10	kJ/mol	NIST Webbook
log10ws	-8.49		Estimated Solubility Method
log10ws	-8.49		Aqueous Solubility Prediction Method
logp	5.640		Crippen Method
mcvol	195.360	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	442.56		NIST Webbook
rinpol	442.80		NIST Webbook
rinpol	443.20		NIST Webbook
rinpol	444.20		NIST Webbook
rinpol	443.60		NIST Webbook
rinpol	443.19		NIST Webbook
rinpol	444.06		NIST Webbook

rinpol	443.05		NIST Webbook
rinpol	441.79		NIST Webbook
rinpol	442.28		NIST Webbook
rinpol	442.77		NIST Webbook
rinpol	437.80		NIST Webbook
rinpol	443.60		NIST Webbook
rinpol	444.60		NIST Webbook
rinpol	430.80		NIST Webbook
rinpol	444.60		NIST Webbook
rinpol	442.72		NIST Webbook
rinpol	444.06		NIST Webbook
rinpol	440.04		NIST Webbook
rinpol	444.02		NIST Webbook
rinpol	442.56		NIST Webbook
rinpol	2708.00		NIST Webbook
rinpol	444.65		NIST Webbook
rinpol	444.02		NIST Webbook
rinpol	444.06		NIST Webbook
rinpol	444.65		NIST Webbook
rinpol	442.80		NIST Webbook
rinpol	436.00		NIST Webbook
rinpol	442.60		NIST Webbook
rinpol	442.80		NIST Webbook
rinpol	443.60		NIST Webbook
rinpol	442.80		NIST Webbook
rinpol	441.09		NIST Webbook
rinpol	441.16		NIST Webbook
rinpol	443.44		NIST Webbook
rinpol	444.60		NIST Webbook
rinpol	442.56		NIST Webbook
rinpol	444.02		NIST Webbook
rinpol	444.43		NIST Webbook
rinpol	2781.00		NIST Webbook
rinpol	442.56		NIST Webbook
rinpol	2789.00		NIST Webbook
rinpol	2780.00		NIST Webbook
rinpol	2789.11		NIST Webbook
rinpol	2722.00		NIST Webbook
rinpol	2706.00		NIST Webbook
rinpol	2702.00		NIST Webbook
rinpol	2761.00		NIST Webbook
rinpol	430.60		NIST Webbook
rinpol	440.48		NIST Webbook
tb	753.00	K	NIST Webbook

tb	753.20	K	NIST Webbook
tc	1030.60	K	Joback Method
tf	489.65	K	Aqueous Solubility Prediction Method
tf	490.00	K	NIST Webbook
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.00	J/mol×K	1030.60	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
cpg	584.31	J/mol×K	986.64	Joback Method
cpg	521.16	J/mol×K	766.84	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	0.0027980	Pa×s	599.76	Joback Method
dvisc	0.0029976	Pa×s	557.99	Joback Method
dvisc	0.0022895	Pa×s	766.84	Joback Method
dvisc	0.0032474	Pa×s	516.22	Joback Method
hfust	32.40	kJ/mol	489.70	NIST Webbook
hfust	27.50	kJ/mol	490.60	NIST Webbook
hsubt	130.00	kJ/mol	396.50	NIST Webbook
hvapt	88.50	kJ/mol	398.00	NIST Webbook
pvap	2.33e-07	kPa	320.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.55e-05	kPa	370.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	5.70e-08	kPa	310.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.74e-04	kPa	390.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	8.19e-04	kPa	400.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.70e-03	kPa	410.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.39e-03	kPa	420.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.45e-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	0.09	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	0.22	kPa	500.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.33	kPa	510.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	1.24e-08	kPa	300.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	9.26e-09	kPa	298.15	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.49e-05	kPa	360.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	8.78e-06	kPa	350.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.87e-06	kPa	340.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	8.57e-07	kPa	330.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.61e-04	kPa	380.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C207089&Units=SI
Determination of Henry's Law Constant Using Diffusion in Air and Water Boundary Layers:	https://www.doi.org/10.1021/je300954s
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	https://www.doi.org/10.1021/je800300x
McGowan Method:	
Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
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

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