

# 11H-Benzo[b]fluorene

<b>Other names:</b>	2,3-Benzfluorene 2,3-Benzofluorene benzo[b]fluorene
<b>Inchi:</b>	InChI=1S/C17H12/c1-2-6-13-11-17-15(9-12(13)5-1)10-14-7-3-4-8-16(14)17/h1-9,11H,10
<b>InchiKey:</b>	HAPOJKSPCGLOOD-UHFFFAOYSA-N
<b>Formula:</b>	C17H12
<b>SMILES:</b>	<chem>c1ccc2c(c1)Cc1cc3ccccc3cc1-2</chem>
<b>Mol. weight [g/mol]:</b>	216.28
<b>CAS:</b>	243-17-4

## Physical Properties

Property code	Value	Unit	Source
gf	487.50	kJ/mol	Joback Method
hf	340.97	kJ/mol	Joback Method
hfus	24.98	kJ/mol	Joback Method
hvap	97.50 ± 3.90	kJ/mol	NIST Webbook
log10ws	-8.04		Aqueous Solubility Prediction Method
logp	4.411		Crippen Method
mcvol	172.550	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
tb	674.20	K	NIST Webbook
tb	674.50 ± 0.50	K	NIST Webbook
tc	937.21	K	Joback Method
tf	481.50 ± 0.50	K	NIST Webbook
tf	489.70 ± 0.40	K	NIST Webbook
tf	483.45 ± 1.00	K	NIST Webbook
vc	0.667	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.14	J/mol×K	764.74	Joback Method
cpg	479.68	J/mol×K	807.86	Joback Method

cpg	491.43	J/mol×K	850.98	Joback Method
cpg	502.61	J/mol×K	894.10	Joback Method
cpg	513.42	J/mol×K	937.21	Joback Method
cpg	438.86	J/mol×K	678.51	Joback Method
cpg	453.60	J/mol×K	721.63	Joback Method
dvisc	0.0011386	Paxs	596.90	Joback Method
dvisc	0.0010415	Paxs	637.70	Joback Method
dvisc	0.0014198	Paxs	515.28	Joback Method
dvisc	0.0016313	Paxs	474.48	Joback Method
dvisc	0.0019238	Paxs	433.67	Joback Method
dvisc	0.0009629	Paxs	678.51	Joback Method
dvisc	0.0012612	Paxs	556.09	Joback Method
hfust	23.40	kJ/mol	489.70	NIST Webbook
hfust	23.40	kJ/mol	489.70	NIST Webbook
hfust	23.40	kJ/mol	489.70	NIST Webbook
hsubt	111.20	kJ/mol	383.00	NIST Webbook
hsubt	119.30 ± 1.30	kJ/mol	371.00	NIST Webbook
hvapt	84.70	kJ/mol	398.00	NIST Webbook
pvap	0.19	kPa	450.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.00	kPa	490.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.69	kPa	480.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.00	kPa	510.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	0.46	kPa	470.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.30	kPa	460.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.12	kPa	440.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.43	kPa	500.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.07	kPa	430.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.04	kPa	420.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.02	kPa	410.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	0.01	kPa	400.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.63e-03	kPa	390.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.29e-03	kPa	380.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.56e-03	kPa	370.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.97e-04	kPa	360.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.94e-04	kPa	350.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.16e-04	kPa	340.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	1.47e-05	kPa	320.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.60e-06	kPa	310.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.31e-06	kPa	300.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.03e-06	kPa	298.15	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.30e-05	kPa	330.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
sfust	47.80	J/molxK	489.70	NIST Webbook

## Sources

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C243174&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**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](https://en.wikipedia.org/wiki/Joback_method)

**Aqueous Solubility Prediction Method:**

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>sfust:</b>	Entropy of fusion at a given temperature
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/74-486-1/11H-Benzo-b-fluorene.pdf>

Generated by Cheméo on 2025-01-15 18:58:38.303998973 +0000 UTC m=+175734.150924604.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.