Benzo[b]triphenylene

Other names:	1,2,3,4-Dibenzanthracene
	1,2:3,4-dibenzanthracene
	1,2:3,4-dibenzoanthracene
	2,3-Benztriphenylene
	2,3-benzotriphenylene
	Db(a,c)A
	dibenz[a,c]anthracene
	dibenzo[a,c]anthracene
	naphtho-2',3':9,10-phenanthrene
Inchi:	InChI=1S/C22H14/c1-2-8-16-14-22-20-12-6-4-10-18(20)17-9-3-5-11-19(17)21(22)13-15(1
InchiKey:	RAASUWZPTOJQAY-UHFFFAOYSA-N
Formula:	C22H14
SMILES:	c1ccc2cc3c4ccccc4c4ccccc4c3cc2c1
Mol. weight [g/mol]:	278.35
CAS:	215-58-7

Physical Properties

Property code	Value	Unit	Source
gf	644.48	kJ/mol	Joback Method
hf	331.00 ± 11.00	kJ/mol	NIST Webbook
hfs	184.80 ± 8.70	kJ/mol	NIST Webbook
hfus	33.69	kJ/mol	Joback Method
hsub	159.00 ± 6.00	kJ/mol	NIST Webbook
hsub	145.90 ± 6.00	kJ/mol	NIST Webbook
hsub	159.00 ± 6.00	kJ/mol	NIST Webbook
hvap	132.30 ± 1.80	kJ/mol	NIST Webbook
ie	7.43	eV	NIST Webbook
ie	7.61	eV	NIST Webbook
ie	7.60	eV	NIST Webbook
ie	7.39 ± 0.02	eV	NIST Webbook
ie	7.39	eV	NIST Webbook
ie	7.44	eV	NIST Webbook
ie	7.39	eV	NIST Webbook
ie	7.44 ± 0.04	eV	NIST Webbook
ie	7.35 ± 0.01	eV	NIST Webbook
log10ws	-8.69		Crippen Method
logp	6.299		Crippen Method

mcvol	219.240	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinpol	3089.00		NIST Webbook
rinpol	495.00		NIST Webbook
rinpol	495.05		NIST Webbook
rinpol	495.01		NIST Webbook
rinpol	498.34		NIST Webbook
rinpol	3142.00		NIST Webbook
rinpol	3142.00		NIST Webbook
rinpol	3089.00		NIST Webbook
rinpol	500.25		NIST Webbook
rinpol	3114.00		NIST Webbook
rinpol	3080.00		NIST Webbook
rinpol	3151.00		NIST Webbook
rinpol	3099.00		NIST Webbook
rinpol	3142.00		NIST Webbook
rinpol	496.60		NIST Webbook
rinpol	495.90		NIST Webbook
rinpol	495.01		NIST Webbook
rinpol	495.10		NIST Webbook
rinpol	495.92		NIST Webbook
rinpol	495.10		NIST Webbook
rinpol	490.13		NIST Webbook
rinpol	496.20		NIST Webbook
rinpol	497.09		NIST Webbook
rinpol	495.01		NIST Webbook
rinpol	483.27		NIST Webbook
rinpol	483.27		NIST Webbook
rinpol	495.56		NIST Webbook
rinpol	495.00		NIST Webbook
rinpol	495.10		NIST Webbook
rinpol	3103.00		NIST Webbook
rinpol	493.39		NIST Webbook
tb	791.20	K	NIST Webbook
tc	1089.89	K	Joback Method
tf	478.00 ± 4.00	K	NIST Webbook
tf	477.00 ± 4.00	K	NIST Webbook
tf	478.20 ± 4.00	K	NIST Webbook
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.04	J/mol×K	1089.89	Joback Method
cpg	622.45	J/mol×K	865.23	Joback Method
cpg	636.52	J/mol×K	910.16	Joback Method
cpg	650.13	J/mol×K	955.09	Joback Method
cpg	663.56	J/mol×K	1000.03	Joback Method
cpg	677.10	J/mol×K	1044.96	Joback Method
cpg	607.64	J/mol×K	820.30	Joback Method
dvisc	0.0012090	Pa×s	772.33	Joback Method
dvisc	0.0013254	Pa×s	724.36	Joback Method
dvisc	0.0014719	Pa×s	676.39	Joback Method
dvisc	0.0016611	Pa×s	628.42	Joback Method
dvisc	0.0019125	Pa×s	580.45	Joback Method
dvisc	0.0011148	Pa×s	820.30	Joback Method
dvisc	0.0022584	Pa×s	532.48	Joback Method
hfust	25.82	kJ/mol	553.50	NIST Webbook
hfust	25.82	kJ/mol	553.50	NIST Webbook
hsubt	135.00	kJ/mol	383.00	NIST Webbook
hvapt	97.50	kJ/mol	398.00	NIST Webbook
pvap	1.09e-08	kPa	320.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.50e-06	kPa	370.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.21e-09	kPa	310.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	4.65e-05	kPa	390.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.13e-04	kPa	400.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.58e-04	kPa	410.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	5.59e-04	kPa	420.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.15e-03	kPa	430.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.27e-03	kPa	440.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.29e-03	kPa	450.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	7.79e-03	kPa	460.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.01	kPa	470.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.02	kPa	480.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.04	kPa	490.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.06	kPa	500.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.09	kPa	510.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.93e-10	kPa	300.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	2.81e-10	kPa	298.15	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.17e-06	kPa	360.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.70e-07	kPa	350.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.88e-07	kPa	340.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.79e-08	kPa	330.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.80e-05	kPa	380.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C215587&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
McGowan Method:	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
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