Benzo[ghi]perylene

Other names:	1,12-Benzoperylene
	1,12-Benzperylene
	191-24-2
	Benzo-1,12-perylene
Inchi:	InChI=1S/C22H12/c1-3-13-7-9-15-11-12-16-10-8-14-4-2-6-18-17(5-1)19(13)21(15)22(16)
InchiKey:	GYFAGKUZYNFMBN-UHFFFAOYSA-N
Formula:	C22H12
SMILES:	c1cc2ccc3ccc4ccc5cccc6c(c1)c2c3c4c56
Mol. weight [g/mol]:	276.33
CAS:	191-24-2

Physical Properties

Property code	Value	Unit	Source
affp	876.00	kJ/mol	NIST Webbook
affp	877.80	kJ/mol	NIST Webbook
basg	845.20	kJ/mol	NIST Webbook
basg	850.60	kJ/mol	NIST Webbook
ea	0.42 ± 0.10	eV	NIST Webbook
gf	729.98	kJ/mol	Joback Method
hf	557.67	kJ/mol	Joback Method
hfus	16.30	kJ/mol	Solid vapor pressure for five heavy PAHs via the Knudsen effusion method
hsub	126.00	kJ/mol	NIST Webbook
hvap	128.90 ± 1.50	kJ/mol	NIST Webbook
ie	7.15	eV	NIST Webbook
ie	7.35	eV	NIST Webbook
ie	7.20 ± 0.05	eV	NIST Webbook
ie	7.15	eV	NIST Webbook
ie	7.13	eV	NIST Webbook
ie	7.19 ± 0.01	eV	NIST Webbook
ie	7.17 ± 0.02	eV	NIST Webbook
ie	7.15	eV	NIST Webbook
log10ws	-9.03		Aqueous Solubility Prediction Method
log10ws	-9.02		Estimated Solubility Method
logp	6.328		Crippen Method

mcvol	208.380	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	500.00		NIST Webbook
rinpol	501.38		NIST Webbook
rinpol	500.00		NIST Webbook
rinpol	501.32		NIST Webbook
rinpol	500.00		NIST Webbook
rinpol	500.00		NIST Webbook
rinpol	501.92		NIST Webbook
rinpol	500.29		NIST Webbook
rinpol	500.00		NIST Webbook
rinpol	502.84		NIST Webbook
rinpol	501.35		NIST Webbook
rinpol	500.00		NIST Webbook
rinpol	501.38		NIST Webbook
rinpol	500.00		NIST Webbook
rinpol	501.59		NIST Webbook
rinpol	500.29		NIST Webbook
rinpol	501.32		NIST Webbook
rinpol	498.90		NIST Webbook
rinpol	501.64		NIST Webbook
rinpol	501.32		NIST Webbook
rinpol	501.38		NIST Webbook
rinpol	501.64		NIST Webbook
rinpol	501.30		NIST Webbook
rinpol	501.32		NIST Webbook
rinpol	499.61		NIST Webbook
rinpol	500.29		NIST Webbook
rinpol	502.90		NIST Webbook
rinpol	501.30		NIST Webbook
rinpol	502.90		NIST Webbook
rinpol	502.90		NIST Webbook
rinpol	500.20		NIST Webbook
rinpol	500.29		NIST Webbook
rinpol	500.29		NIST Webbook
rinpol	501.88		NIST Webbook
rinpol	501.32		NIST Webbook
rinpol	500.29		NIST Webbook
rinpol	501.90		NIST Webbook
rinpol	501.32		NIST Webbook
rinpol	499.69		NIST Webbook
rinpol	500.00		NIST Webbook
rinpol	502.80		NIST Webbook
rinpol	501.32		NIST Webbook

rinpol	526.92		NIST Webbook
rinpol	501.01		NIST Webbook
rinpol	501.32		NIST Webbook
rinpol	3144.00		NIST Webbook
rinpol	3115.00		NIST Webbook
rinpol	3168.40		NIST Webbook
rinpol	3160.00		NIST Webbook
rinpol	3146.00		NIST Webbook
rinpol	501.32		NIST Webbook
rinpol	3185.00		NIST Webbook
rinpol	3144.00		NIST Webbook
rinpol	3149.00		NIST Webbook
rinpol	3160.00		NIST Webbook
rinpol	3131.80		NIST Webbook
rinpol	3124.00		NIST Webbook
rinpol	3144.00		NIST Webbook
rinpol	3150.00		NIST Webbook
rinpol	3124.00		NIST Webbook
rinpol	3185.00		NIST Webbook
rinpol	3185.00		NIST Webbook
rinpol	3168.40		NIST Webbook
rinpol	3150.10		NIST Webbook
rinpol	3137.00		NIST Webbook
rinpol	3124.00		NIST Webbook
rinpol	3122.00		NIST Webbook
rinpol	3115.00		NIST Webbook
rinpol	3146.00		NIST Webbook
rinpol	501.30		NIST Webbook
rinpol	502.60		NIST Webbook
tb	828.86	K	Joback Method
tc	1092.51	K	Joback Method
tf	553.00 ± 0.20	K	NIST Webbook
tf	554.20 ± 0.40	K	NIST Webbook
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.06	J/mol×K	828.86	Joback Method
cpg	586.21	J/mol×K	872.80	Joback Method
cpg	599.31	J/mol×K	916.74	Joback Method

cpg	612.69	J/mol×K	960.68	Joback Method
cpg	626.73	J/mol×K	1004.62	Joback Method
cpg	641.76	J/mol×K	1048.57	Joback Method
cpg	658.14	J/mol×K	1092.51	Joback Method
dvisc	0.0083814	Pa×s	590.26	Joback Method
dvisc	0.0081674	Pa×s	789.09	Joback Method
dvisc	0.0082008	Pa×s	749.33	Joback Method
dvisc	0.0081374	Pa×s	828.86	Joback Method
dvisc	0.0082799	Pa×s	669.79	Joback Method
dvisc	0.0083273	Pa×s	630.03	Joback Method
dvisc	0.0082380	Pa×s	709.56	Joback Method
hfust	17.37	kJ/mol	554.20	NIST Webbook
hfust	17.37	kJ/mol	554.20	NIST Webbook
hsubt	129.90	kJ/mol	383.00	NIST Webbook
hsubt	127.80	kJ/mol	428.50	NIST Webbook
hsubt	135.10	kJ/mol	480.00	NIST Webbook
hsubt	125.50	kJ/mol	478.00	NIST Webbook
hvapt	96.10	kJ/mol	398.00	NIST Webbook
pvap	4.07e-03	kPa	450.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.03	kPa	490.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.08	kPa	510.00	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	0.01	kPa	470.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	7.27e-03	kPa	460.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.05	kPa	500.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.19e-03	kPa	440.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.13e-03	kPa	430.00	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	2.63e-04	kPa	410.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	1.18e-04	kPa	400.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.98e-05	kPa	390.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.98e-05	kPa	380.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	7.35e-06	kPa	370.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.54e-06	kPa	360.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	8.09e-07	kPa	350.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.36e-07	kPa	340.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	1.50e-08	kPa	320.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.18e-09	kPa	310.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	5.96e-10	kPa	300.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.31e-10	kPa	298.15	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.26e-08	kPa	330.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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

Legend

affp:	Proton affinity
basg:	Gas basicity
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
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