Dibenz[a,h]anthracene

Other names:	1,2,5,6-DBA
	1,2,5,6-Dibenzanthraceen
	1,2,5,6-Dibenzanthracene
	1,2:5,6-Dibenz(a)anthracene
	1,2:5,6-benzanthracene
	1,2:5,6-dibenz[a]anthracene
	1,2:5,6-dibenzanthracene
	1,2:5,6-dibenzoanthracene
	DB(a,h)A
	DBA
	Dibenz(a,h)antracene
	NSC 22433
	Rcra waste number U063
	dibenzo[a,h]anthracene
Inchi:	InChI=1S/C22H14/c1-3-7-19-15(5-1)9-11-17-14-22-18(13-21(17)19)12-10-16-6-2-4-8-20(
InchiKey:	LHRCREOYAASXPZ-UHFFFAOYSA-N
Formula:	C22H14
SMILES:	c1ccc2c(c1)ccc1cc3c(ccc4ccccc43)cc12
Mol. weight [g/mol]:	278.35
CAS:	53-70-3

Physical Properties

Property code	Value	Unit	Source
ea	0.59 ± 0.01	eV	NIST Webbook
gf	644.48	kJ/mol	Joback Method
hf	328.00 ± 11.00	kJ/mol	NIST Webbook
hfs	179.00 ± 10.00	kJ/mol	NIST Webbook
hfus	24.50	kJ/mol	Solid vapor pressure for five heavy PAHs via the Knudsen effusion method
hsub	148.90 ± 4.20	kJ/mol	NIST Webbook
hsub	162.00 ± 6.00	kJ/mol	NIST Webbook
hsub	142.00	kJ/mol	NIST Webbook
hsub	162.00 ± 6.00	kJ/mol	NIST Webbook
hvap	131.10 ± 1.40	kJ/mol	NIST Webbook
ie	7.38 ± 0.04	eV	NIST Webbook
ie	7.39 ± 0.01	eV	NIST Webbook

ie	7.41	eV	NIST Webbook
ie	7.38	eV	NIST Webbook
ie	7.42	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
ie	7.58	eV	NIST Webbook
ie	7.57	eV	NIST Webbook
ie	7.60 ± 0.10	eV	NIST Webbook
ie	7.38 ± 0.02	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	490.31		NIST Webbook
rinpol	3114.00		NIST Webbook
rinpol	3080.00		NIST Webbook
rinpol	3060.00		NIST Webbook
rinpol	3108.00		NIST Webbook
rinpol	3096.00		NIST Webbook
rinpol	3099.00		NIST Webbook
rinpol	3137.00		NIST Webbook
rinpol	495.40		NIST Webbook
rinpol	496.10		NIST Webbook
rinpol	495.45		NIST Webbook
rinpol	494.50		NIST Webbook
rinpol	494.91		NIST Webbook
rinpol	495.92		NIST Webbook
rinpol	493.42		NIST Webbook
rinpol	3095.00		NIST Webbook
rinpol	493.34		NIST Webbook
rinpol	493.51		NIST Webbook
rinpol	492.15		NIST Webbook
rinpol	488.20		NIST Webbook
rinpol	3089.00		NIST Webbook
rinpol	492.41		NIST Webbook
rinpol	495.92		NIST Webbook
rinpol	491.01		NIST Webbook
rinpol	496.20		NIST Webbook
rinpol	495.45		NIST Webbook
rinpol	495.89		NIST Webbook
rinpol	495.45		NIST Webbook
rinpol	495.89		NIST Webbook
rinpol	495.92		NIST Webbook
rinpol	499.00		NIST Webbook
rinpol	489.00		NIST Webbook

rinpol	491.45		NIST Webbook
rinpol	491.82		NIST Webbook
rinpol	494.50		NIST Webbook
rinpol	495.50		NIST Webbook
rinpol	499.00		NIST Webbook
rinpol	494.50		NIST Webbook
rinpol	491.85		NIST Webbook
rinpol	491.99		NIST Webbook
rinpol	496.20		NIST Webbook
rinpol	3137.00		NIST Webbook
rinpol	499.02		NIST Webbook
rinpol	495.45		NIST Webbook
rinpol	3137.00		NIST Webbook
rinpol	493.09		NIST Webbook
rinpol	493.92		NIST Webbook
rinpol	495.45		NIST Webbook
rinpol	501.23		NIST Webbook
rinpol	495.45		NIST Webbook
rinpol	490.31		NIST Webbook
rinpol	495.66		NIST Webbook
rinpol	3089.00		NIST Webbook
rinpol	495.51		NIST Webbook
rinpol	495.66		NIST Webbook
rinpol	494.19		NIST Webbook
tb	797.20	K	NIST Webbook
tc	1089.89	K	Joback Method
tf	533.15 ± 2.00	K	NIST Webbook
tf	543.00 ± 2.00	K	NIST Webbook
tf	537.65 ± 1.00	K	NIST Webbook
tf	535.00 ± 5.00	K	NIST Webbook
tf	544.20 ± 0.40	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	607.64	J/mol×K	820.30	Joback Method
cpg	663.56	J/mol×K	1000.03	Joback Method

cpg	677.10	J/mol×K	1044.96	Joback Method
cpg	650.13	J/mol×K	955.09	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	0.0011148	Pa×s	820.30	Joback Method
dvisc	0.0022584	Pa×s	532.48	Joback Method
dvisc	0.0016611	Pa×s	628.42	Joback Method
dvisc	0.0019125	Pa×s	580.45	Joback Method
hfust	28.40	kJ/mol	539.70	NIST Webbook
hfust	31.16	kJ/mol	544.20	NIST Webbook
hfust	31.16	kJ/mol	544.20	NIST Webbook
hsubt	141.80	kJ/mol	459.50	NIST Webbook
hvapt	99.40	kJ/mol	398.00	NIST Webbook
pvap	4.47e-03	kPa	450.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.38e-03	kPa	440.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.21e-03	kPa	430.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	8.07e-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	0.10	kPa	510.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	5.93e-04	kPa	420.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.75e-04	kPa	410.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	1.21e-04	kPa	400.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	5.03e-05	kPa	390.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.96e-05	kPa	380.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	7.14e-06	kPa	370.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.41e-06	kPa	360.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	7.49e-07	kPa	350.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.13e-07	kPa	340.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	5.47e-08	kPa	330.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.26e-08	kPa	320.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.59e-09	kPa	310.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.67e-10	kPa	300.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.35e-10	kPa	298.15	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53703&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
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