Pentacene

Other names:	2,3,6,7-Dibenzanthracene
	2,3:6,7-dibenzanthracene
	benzo[b]naphthacene
	lin-dibenzanthracene
	lin-naphthoanthracene
Inchi:	InChI=1S/C22H14/c1-2-6-16-10-20-14-22-12-18-8-4-3-7-17(18)11-21(22)13-19(20)9-15(1
InchiKey:	SLIUAWYAILUBJU-UHFFFAOYSA-N
Formula:	C22H14
SMILES:	c1ccc2cc3cc4cc5ccccc5cc4cc3cc2c1
Mol. weight [g/mol]:	278.35
CAS:	135-48-8

Physical Properties

Property code	Value	Unit	Source
basg	836.00	kJ/mol	NIST Webbook
ea	1.39 ± 0.04	eV	NIST Webbook
gf	644.48	kJ/mol	Joback Method
hf	468.99	kJ/mol	Joback Method
hfus	33.69	kJ/mol	Joback Method
hsub	158.00	kJ/mol	NIST Webbook
hsub	184.00 ± 10.00	kJ/mol	NIST Webbook
hsub	184.00 ± 10.00	kJ/mol	NIST Webbook
hvap	75.39	kJ/mol	Joback Method
ie	6.61	eV	NIST Webbook
ie	6.64	eV	NIST Webbook
ie	6.74 ± 0.01	eV	NIST Webbook
ie	6.60 ± 0.10	eV	NIST Webbook
ie	6.61	eV	NIST Webbook
ie	6.62	eV	NIST Webbook
ie	6.23	eV	NIST Webbook
ie	6.61 ± 0.02	eV	NIST Webbook
ie	6.63 ± 0.05	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
rhoc	345.43 ± 10.02	kg/m3	NIST Webbook

rinpol	486.81		NIST Webbook
rinpol	483.80		NIST Webbook
rinpol	486.81		NIST Webbook
rinpol	486.80		NIST Webbook
rinpol	483.80		NIST Webbook
rinpol	486.81		NIST Webbook
rinpol	486.81		NIST Webbook
tb	820.30	K	Joback Method
tc	1089.89	K	Joback Method
tf	544.00 ± 3.00	K	NIST Webbook
tf	544.00 ± 2.00	K	NIST Webbook
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.45	J/mol×K	865.23	Joback Method
cpg	691.04	J/mol×K	1089.89	Joback Method
cpg	677.10	J/mol×K	1044.96	Joback Method
cpg	663.56	J/mol×K	1000.03	Joback Method
cpg	650.13	J/mol×K	955.09	Joback Method
cpg	607.64	J/mol×K	820.30	Joback Method
cpg	636.52	J/mol×K	910.16	Joback Method
cps	366.00	J/mol×K	350.00	Heat Capacities of Tetracene and Pentacene
cps	346.50	J/mol×K	329.60	Heat Capacities of Tetracene and Pentacene
cps	345.70	J/mol×K	329.60	Heat Capacities of Tetracene and Pentacene
cps	332.10	J/mol×K	319.40	Heat Capacities of Tetracene and Pentacene
cps	344.50	J/mol×K	329.60	Heat Capacities of Tetracene and Pentacene
cps	356.20	J/mol×K	339.80	Heat Capacities of Tetracene and Pentacene
cps	354.90	J/mol×K	339.80	Heat Capacities of Tetracene and Pentacene
cps	355.10	J/mol×K	339.80	Heat Capacities of Tetracene and Pentacene

cps	365.50	J/mol×K	350.00	Heat Capacities of Tetracene and Pentacene
cps	367.20	J/mol×K	350.00	Heat Capacities of Tetracene and Pentacene
cps	264.50	J/mol×K	258.10	Heat Capacities of Tetracene and Pentacene
cps	265.50	J/mol×K	258.10	Heat Capacities of Tetracene and Pentacene
cps	267.20	J/mol×K	258.10	Heat Capacities of Tetracene and Pentacene
cps	275.70	J/mol×K	268.30	Heat Capacities of Tetracene and Pentacene
cps	277.20	J/mol×K	268.30	Heat Capacities of Tetracene and Pentacene
cps	277.10	J/mol×K	268.30	Heat Capacities of Tetracene and Pentacene
cps	332.50	J/mol×K	319.40	Heat Capacities of Tetracene and Pentacene
cps	287.10	J/mol×K	278.50	Heat Capacities of Tetracene and Pentacene
cps	287.50	J/mol×K	278.50	Heat Capacities of Tetracene and Pentacene
cps	299.70	J/mol×K	288.70	Heat Capacities of Tetracene and Pentacene
cps	299.70	J/mol×K	288.70	Heat Capacities of Tetracene and Pentacene
cps	299.20	J/mol×K	288.70	Heat Capacities of Tetracene and Pentacene
cps	311.60	J/mol×K	298.90	Heat Capacities of Tetracene and Pentacene
cps	311.50	J/mol×K	298.90	Heat Capacities of Tetracene and Pentacene
cps	311.00	J/mol×K	298.90	Heat Capacities of Tetracene and Pentacene
cps	322.10	J/mol×K	309.10	Heat Capacities of Tetracene and Pentacene
cps	322.40	J/mol×K	309.10	Heat Capacities of Tetracene and Pentacene

cps	322.30	J/mol×K	309.10	Heat Capacities of Tetracene and Pentacene
cps	288.90	J/mol×K	278.50	Heat Capacities of Tetracene and Pentacene
cps	333.20	J/mol×K	319.40	Heat Capacities of Tetracene and Pentacene
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
dvisc	0.0012090	Pa×s	772.33	Joback Method
dvisc	0.0011148	Pa×s	820.30	Joback Method
dvisc	0.0013254	Pa×s	724.36	Joback Method
dvisc	0.0014719	Pa×s	676.39	Joback Method
hsubt	157.70	kJ/mol	505.00	NIST Webbook
hsubt	154.00 ± 5.00	kJ/mol	510.00	NIST Webbook
hsubt	157.00 ± 14.00	kJ/mol	463.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C135488&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Heat Capacities of Tetracene and Pentacene:	https://www.doi.org/10.1021/je800382b
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

basg:	Gas basicity
cpg:	Ideal gas heat capacity
cps:	Solid phase 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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rhoc:	Critical density
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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