Perylene

Other names:	Dibenz[de,kl]anthracene
	Peri-Dinaphthalene
	Perilene
	«alpha»-Perylene
	Â«alphaÂ»-Perylene
Inchi:	InChI=1S/C20H12/c1-5-13-6-2-11-17-18-12-4-8-14-7-3-10-16(20(14)18)15(9-1)19(13)17/
InchiKey:	CSHWQDPOILHKBI-UHFFFAOYSA-N
Formula:	C20H12
SMILES:	c1cc2cccc3c4cccc5cccc(c(c1)c23)c54
Mol. weight [g/mol]:	252.31
CAS:	198-55-0

Physical Properties

Property code	Value	Unit	Source
affp	887.40	kJ/mol	NIST Webbook
affp	888.60	kJ/mol	NIST Webbook
basg	859.40	kJ/mol	NIST Webbook
basg	859.60	kJ/mol	NIST Webbook
chs	-9767.97 ± 0.46	kJ/mol	NIST Webbook
chs	-9754.00 ± 61.00	kJ/mol	NIST Webbook
ea	0.97 ± 0.01	eV	NIST Webbook
ea	0.35 ± 0.10	eV	NIST Webbook
ea	0.99 ± 0.04	eV	NIST Webbook
gf	621.88	kJ/mol	Joback Method
hf	318.30 ± 3.70	kJ/mol	NIST Webbook
hfs	182.40 ± 2.70	kJ/mol	NIST Webbook
hfs	182.70 ± 0.46	kJ/mol	NIST Webbook
hfus	31.48	kJ/mol	Joback Method
hsub	145.20 ± 2.50	kJ/mol	NIST Webbook
hsub	125.50 ± 4.20	kJ/mol	NIST Webbook
hsub	135.90 ± 2.60	kJ/mol	NIST Webbook
hvap	119.50	kJ/mol	NIST Webbook
hvap	123.10 ± 1.70	kJ/mol	NIST Webbook
ie	6.90 ± 0.01	eV	NIST Webbook
ie	7.15	eV	NIST Webbook
ie	7.03	eV	NIST Webbook
ie	6.96 ± 0.00	eV	NIST Webbook

ie	7.10	eV	NIST Webbook
ie	7.00 ± 0.01	eV	NIST Webbook
ie	7.10 ± 0.10	eV	NIST Webbook
ie	7.10	eV	NIST Webbook
ie	6.85	eV	NIST Webbook
ie	7.11	eV	NIST Webbook
ie	6.83	eV	NIST Webbook
ie	6.97	eV	NIST Webbook
ie	6.97	eV	NIST Webbook
ie	6.96 ± 0.00	eV	NIST Webbook
ie	7.06	eV	NIST Webbook
log10ws	-8.79		Aqueous Solubility Prediction Method
log10ws	-8.80		Estimated Solubility Method
logp	5.737		Crippen Method
mcvol	195.360	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	457.17		NIST Webbook
rinpol	2814.00		NIST Webbook
rinpol	454.90		NIST Webbook
rinpol	457.50		NIST Webbook
rinpol	456.80		NIST Webbook
rinpol	457.70		NIST Webbook
rinpol	456.22		NIST Webbook
rinpol	456.30		NIST Webbook
rinpol	457.93		NIST Webbook
rinpol	457.63		NIST Webbook
rinpol	457.02		NIST Webbook
rinpol	455.95		NIST Webbook
rinpol	456.17		NIST Webbook
rinpol	452.00		NIST Webbook
rinpol	457.17		NIST Webbook
rinpol	458.36		NIST Webbook
rinpol	458.21		NIST Webbook
rinpol	456.59		NIST Webbook
rinpol	457.63		NIST Webbook
rinpol	451.27		NIST Webbook
rinpol	454.60		NIST Webbook
rinpol	2852.00		NIST Webbook
rinpol	456.22		NIST Webbook
rinpol	457.98		NIST Webbook
rinpol	457.17		NIST Webbook
rinpol	2781.00		NIST Webbook
rinpol	457.98		NIST Webbook

rinpol	457.50	NIST Webbook
rinpol	454.11	NIST Webbook
rinpol	456.20	NIST Webbook
rinpol	456.30	NIST Webbook
rinpol	457.50	NIST Webbook
rinpol	456.30	NIST Webbook
rinpol	454.50	NIST Webbook
rinpol	456.22	NIST Webbook
rinpol	457.17	NIST Webbook
rinpol	455.59	NIST Webbook
rinpol	457.45	NIST Webbook
rinpol	456.22	NIST Webbook
rinpol	456.25	NIST Webbook
rinpol	459.60	NIST Webbook
rinpol	453.62	NIST Webbook
rinpol	456.22	NIST Webbook
rinpol	457.98	NIST Webbook
rinpol	2814.00	NIST Webbook
rinpol	456.22	NIST Webbook
rinpol	455.95	NIST Webbook
rinpol	458.21	NIST Webbook
rinpol	457.17	NIST Webbook
rinpol	2837.20	NIST Webbook
rinpol	2795.00	NIST Webbook
rinpol	2815.00	NIST Webbook
rinpol	2847.00	NIST Webbook
rinpol	454.90	NIST Webbook
rinpol	2781.00	NIST Webbook
rinpol	2800.00	NIST Webbook
rinpol	2815.42	NIST Webbook
rinpol	2812.49	NIST Webbook
rinpol	2848.00	NIST Webbook
rinpol	2847.00	NIST Webbook
rinpol	2832.00	NIST Webbook
rinpol	2828.00	NIST Webbook
rinpol	2825.00	NIST Webbook
rinpol	2815.00	NIST Webbook
rinpol	2815.00	NIST Webbook
rinpol	2815.00	NIST Webbook
rinpol	2815.00	NIST Webbook
rinpol	2795.00	NIST Webbook
rinpol	2795.00	NIST Webbook
rinpol	2795.00	NIST Webbook
rinpol	2795.00	NIST Webbook

rinpol	2791.00		NIST Webbook
rinpol	2800.00		NIST Webbook
rinpol	2837.20		NIST Webbook
rinpol	2846.00		NIST Webbook
rinpol	2850.00		NIST Webbook
rinpol	2832.00		NIST Webbook
rinpol	2829.00		NIST Webbook
rinpol	2797.00		NIST Webbook
rinpol	2783.00		NIST Webbook
rinpol	2783.00		NIST Webbook
rinpol	2849.00		NIST Webbook
rinpol	457.63		NIST Webbook
rinpol	2837.00		NIST Webbook
ss	264.60	J/mol×K	NIST Webbook
tb	766.84	K	Joback Method
tc	1030.60	K	Joback Method
tf	549.57	K	Aqueous Solubility Prediction Method
tt	550.95 ± 0.01	K	NIST Webbook
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.01	J/mol×K	942.68	Joback Method
cpg	584.31	J/mol×K	986.64	Joback Method
cpg	534.69	J/mol×K	810.80	Joback Method
cpg	547.49	J/mol×K	854.76	Joback Method
cpg	559.83	J/mol×K	898.72	Joback Method
cpg	597.00	J/mol×K	1030.60	Joback Method
cpg	521.16	J/mol×K	766.84	Joback Method
cps	274.90	J/mol×K	298.15	NIST Webbook
dvisc	0.0025002	Pa×s	683.30	Joback Method
dvisc	0.0022895	Pa×s	766.84	Joback Method
dvisc	0.0023865	Pa×s	725.07	Joback Method
dvisc	0.0032474	Pa×s	516.22	Joback Method
dvisc	0.0029976	Pa×s	557.99	Joback Method
dvisc	0.0027980	Pa×s	599.76	Joback Method
dvisc	0.0026352	Pa×s	641.53	Joback Method
hfust	31.88	kJ/mol	551.00	NIST Webbook
hfust	32.58	kJ/mol	551.29	NIST Webbook

hsubt	121.30	kJ/mol	370.00	NIST Webbook
hsubt	129.60 ± 2.10	kJ/mol	415.00	NIST Webbook
hsubt	139.00	kJ/mol	418.00	NIST Webbook
hsubt	123.20	kJ/mol	383.00	NIST Webbook
hsubt	132.60 ± 3.60	kJ/mol	407.50	NIST Webbook
hvapt	119.52	kJ/mol	298.00	Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons. Liquid-Vapor Pressure Isotope Effects
hvapt	89.90	kJ/mol	398.00	NIST Webbook
psub	3.15e-05	kPa	397.70	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	5.19e-05	kPa	403.70	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	6.67e-05	kPa	405.70	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	7.20e-05	kPa	406.60	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	7.03e-05	kPa	406.80	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method

psub	1.00e-04	kPa	410.50	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	1.02e-04	kPa	411.30	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	1.32e-04	kPa	412.70	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	1.42e-04	kPa	413.40	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	1.48e-04	kPa	414.40	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	1.96e-04	kPa	418.40	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	4.43e-04	kPa	428.60	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	

psub	6.06e-04	kPa	432.40	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	2.15e-05	kPa	393.70	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	1.49e-05	kPa	391.20	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	1.47e-05	kPa	390.50	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	1.37e-05	kPa	390.00	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	4.76e-05	kPa	402.80	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	4.58e-05	kPa	402.20	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	

psub	3.03e-05	kPa	398.30	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method

Sources

Measurement and Correlation of Diffusion Coefficients of Aromatic Compounds at Infinite Dilution in Alkane and Cycloalkane Solvents:	https://www.doi.org/10.1021/je6005604
Solubilities of Organic Semiconductors and Nonsteroidal Anti-inflammatory Drugs in Pure and Mixed Organic Solvents: Measurement and Modeling With Hansen Solubility Parameter:	https://www.doi.org/10.1021/acs.jced.8b00536
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C198550&Units=SI
Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method:	https://www.doi.org/10.1021/je7005133
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Polycyclic Aromatic Hydrocarbons: Liquid-Vapor Pressure Isotope Effects:	https://www.doi.org/10.1021/je800091s
Diffusion Coefficients of Aromatic Compounds at Infinite Dilution in Binary Mixtures at 298.15 K:	https://www.doi.org/10.1021/je060289l
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
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
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
psub:	Sublimation pressure
rinpol:	Non-polar retention indices
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume