Chrysene

Other names:	1,2,5,6-Dibenzonaphthalene
	1,2-Benzophenanthrene
	1,2-Benzphenanthrene
	Benz(a)phenanthrene
	Benzo[a]phenanthrene
	Crysene
	Rcra waste number U050
Inchi:	InChI=1S/C18H12/c1-3-7-15-13(5-1)9-11-18-16-8-4-2-6-14(16)10-12-17(15)18/h1-12H
InchiKey:	WDECIBYCCFPHNR-UHFFFAOYSA-N
Formula:	C18H12
SMILES:	c1ccc2c(c1)ccc1c3ccccc3ccc21
Mol. weight [g/mol]:	228.29
CAS:	218-01-9

Physical Properties

Property code	Value	Unit	Source
affp	840.90	kJ/mol	NIST Webbook
affp	828.90	kJ/mol	NIST Webbook
basg	804.60	kJ/mol	NIST Webbook
basg	810.10	kJ/mol	NIST Webbook
chs	-8943.40 ± 2.10	kJ/mol	NIST Webbook
ea	0.32 ± 0.01	eV	NIST Webbook
ea	0.33	eV	NIST Webbook
ea	0.40 ± 0.01	eV	NIST Webbook
gf	513.78	kJ/mol	Joback Method
hf	268.70 ± 4.70	kJ/mol	NIST Webbook
hfs	145.30 ± 2.20	kJ/mol	NIST Webbook
hfus	26.70	kJ/mol	Joback Method
hsub	131.00 ± 4.00	kJ/mol	NIST Webbook
hsub	123.40 ± 4.20	kJ/mol	NIST Webbook
hsub	131.00 ± 4.00	kJ/mol	NIST Webbook
hvap	106.20	kJ/mol	NIST Webbook
hvap	97.00 ± 1.40	kJ/mol	NIST Webbook
ie	7.80	eV	NIST Webbook
ie	7.59	eV	NIST Webbook
ie	7.59 ± 0.02	eV	NIST Webbook
ie	7.72	eV	NIST Webbook

ie	7.75	eV	NIST Webbook
ie	7.68	eV	NIST Webbook
ie	7.83	eV	NIST Webbook
ie	7.82	eV	NIST Webbook
ie	8.00 ± 0.30	eV	NIST Webbook
ie	7.60 ± 0.01	eV	NIST Webbook
ie	7.59 ± 0.05	eV	NIST Webbook
ie	8.00 ± 0.20	eV	NIST Webbook
ie	7.60 ± 0.03	eV	NIST Webbook
ie	7.60 ± 0.01	eV	NIST Webbook
ie	7.61	eV	NIST Webbook
ie	7.78	eV	NIST Webbook
log10ws	-8.06		Estimated Solubility Method
log10ws	-8.06		Aqueous Solubility Prediction Method
logp	5.146		Crippen Method
mcvol	182.340	ml/mol	McGowan Method
pc	2511.00	kPa	KDB
rinpol	2400.00		NIST Webbook
rinpol	2434.20		NIST Webbook
rinpol	2472.30		NIST Webbook
rinpol	2494.90		NIST Webbook
rinpol	2474.40		NIST Webbook
rinpol	2442.66		NIST Webbook
rinpol	2442.50		NIST Webbook
rinpol	2434.20		NIST Webbook
rinpol	2472.30		NIST Webbook
rinpol	2494.90		NIST Webbook
rinpol	2412.30		NIST Webbook
rinpol	2471.80		NIST Webbook
rinpol	2463.10		NIST Webbook
rinpol	2432.20		NIST Webbook
rinpol	2465.00		NIST Webbook
rinpol	2454.00		NIST Webbook
rinpol	2400.00		NIST Webbook
rinpol	2400.00		NIST Webbook
rinpol	2471.80		NIST Webbook
rinpol	2400.00		NIST Webbook
rinpol	2400.00		NIST Webbook
rinpol	2413.00		NIST Webbook
rinpol	2413.00		NIST Webbook
rinpol	2413.00		NIST Webbook
rinpol	2413.00		NIST Webbook
rinpol	2472.30		NIST Webbook

rinpol	2422.00	NIST Webbook
rinpol	2424.00	NIST Webbook
rinpol	2431.00	NIST Webbook
rinpol	2434.00	NIST Webbook
rinpol	2437.00	NIST Webbook
rinpol	2397.00	NIST Webbook
rinpol	2409.82	NIST Webbook
rinpol	2471.68	NIST Webbook
rinpol	2486.00	NIST Webbook
rinpol	2443.00	NIST Webbook
rinpol	2441.00	NIST Webbook
rinpol	2401.00	NIST Webbook
rinpol	2450.00	NIST Webbook
rinpol	2451.00	NIST Webbook
rinpol	2457.00	NIST Webbook
rinpol	2458.00	NIST Webbook
rinpol	2462.00	NIST Webbook
rinpol	2463.00	NIST Webbook
rinpol	2491.00	NIST Webbook
rinpol	2492.00	NIST Webbook
rinpol	2428.00	NIST Webbook
rinpol	2453.00	NIST Webbook
rinpol	2456.00	NIST Webbook
rinpol	2411.00	NIST Webbook
rinpol	2465.00	NIST Webbook
rinpol	2472.30	NIST Webbook
rinpol	2474.40	NIST Webbook
rinpol	2494.90	NIST Webbook
rinpol	2465.00	NIST Webbook
rinpol	2400.00	NIST Webbook
rinpol	2413.00	NIST Webbook
rinpol	2434.00	NIST Webbook
rinpol	2490.00	NIST Webbook
rinpol	2480.00	NIST Webbook
rinpol	2489.00	NIST Webbook
rinpol	2411.00	NIST Webbook
rinpol	2456.00	NIST Webbook
rinpol	2408.00	NIST Webbook
rinpol	2461.90	NIST Webbook
rinpol	2491.00	NIST Webbook
rinpol	2488.00	NIST Webbook
rinpol	2486.00	NIST Webbook
rinpol	2480.00	NIST Webbook
rinpol	2447.00	NIST Webbook

rinpol	2439.00		NIST Webbook
rinpol	2438.00		NIST Webbook
rinpol	2429.00		NIST Webbook
rinpol	2406.00		NIST Webbook
rinpol	2408.00		NIST Webbook
rinpol	2422.00		NIST Webbook
rinpol	2406.00		NIST Webbook
tb	721.20	K	NIST Webbook
tb	721.15	K	KDB
tc	984.20	K	KDB
tf	527.35 ± 1.00	K	NIST Webbook
tf	529.00 ± 2.00	K	NIST Webbook
tf	529.18	K	Aqueous Solubility Prediction Method
tf	529.20 ± 1.00	K	NIST Webbook
tf	531.40 ± 0.20	K	NIST Webbook
tf	528.90	K	KDB
tf	527.90 ± 0.50	K	NIST Webbook
vc	0.700	m3/kmol	KDB
zc	0.2147950		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.24	J/mol×K	968.39	Joback Method
cpg	482.86	J/mol×K	748.75	Joback Method
cpg	496.51	J/mol×K	792.68	Joback Method
cpg	521.02	J/mol×K	880.54	Joback Method
cpg	532.31	J/mol×K	924.47	Joback Method
cpg	509.15	J/mol×K	836.61	Joback Method
cpg	468.00	J/mol×K	704.82	Joback Method
dvisc	0.0007153	Pa×s	704.82	Joback Method
dvisc	0.0011669	Pa×s	529.73	Joback Method
dvisc	0.0017235	Pa×s	442.18	Joback Method
dvisc	0.0007890	Pa×s	661.05	Joback Method
dvisc	0.0008825	Pa×s	617.27	Joback Method
dvisc	0.0010040	Pa×s	573.50	Joback Method
dvisc	0.0013935	Pa×s	485.95	Joback Method
hfust	3.22	kJ/mol	512.20	NIST Webbook
hfust	26.15	kJ/mol	531.40	NIST Webbook
hfust	23.60	kJ/mol	527.00	NIST Webbook

hfust	26.15	kJ/mol	531.40	NIST Webbook
hsubt	118.80	kJ/mol	383.00	NIST Webbook
hsubt	118.00	kJ/mol	293.00	NIST Webbook
hsubt	119.00	kJ/mol	353.00	NIST Webbook
hsubt	121.40	kJ/mol	385.50	NIST Webbook
hsubt	118.00 ± 4.00	kJ/mol	400.00	NIST Webbook
hvapt	106.18	kJ/mol	298.00	Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons. Liquid-Vapor Pressure Isotope Effects
hvapt	89.60	kJ/mol	398.00	NIST Webbook
psub	2.12e-04	kPa	400.40	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	2.92e-04	kPa	404.90	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	3.06e-04	kPa	405.10	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	3.36e-04	kPa	406.80	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	3.79e-04	kPa	408.60	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method

psub	2.77e-04	kPa	404.80	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	2.54e-04	kPa	403.00	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	1.74e-05	kPa	372.40	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	2.02e-04	kPa	400.00	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	1.58e-04	kPa	398.20	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	1.68e-04	kPa	398.10	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	1.48e-04	kPa	396.10	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	

psub	1.36e-04	kPa	394.20	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	1.03e-04	kPa	393.60	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	7.50e-05	kPa	389.40	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	7.61e-05	kPa	389.20	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	5.37e-05	kPa	385.20	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	3.72e-05	kPa	380.70	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	2.63e-04	kPa	402.80	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	

rhol	1278.44	kg/m3	293.10	KDB
sfust	49.21	J/mol×K	531.40	NIST Webbook
sfust	6.29	J/mol×K	512.20	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44202e+01
Coeff. B	-5.84669e+03
Coeff. C	-1.24711e+02
Temperature range (K), min.	538.15
Temperature range (K), max.	766.15

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.25778e+02
Coeff. B	-1.72689e+04
Coeff. C	-1.49941e+01
Coeff. D	3.01277e-06
Temperature range (K), min.	531.15
Temperature range (K), max.	979.00

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons. Liquid-Vapor Pressure Isotope Effects:	https://www.doi.org/10.1021/je800091s
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Measuring the Solubility of Anthracene and Chrysene in Supercritical Fluid Carbon Dioxide Using Static Solubility Data Directly Interfaced Online to Supercritical Fluid Chromatography:	https://www.doi.org/10.1021/acs.jced.7b00857
Determination of Henry's Law Constant Using Diffusion in Air and Water:	https://www.doi.org/10.1021/je300954s
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method:	https://www.doi.org/10.1021/je7005133
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C218019&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=807
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=807

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
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
psub:	Sublimation pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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