

Pyrene

Other names:	BENZOPHENANTHRENE BETA-PYRENE Benzo[def]phenanthrene Coal tar pitch volatiles:pyrene Pyren benzo(def)phenanthrene «beta»-Pyrene Â«betaÂ»-Pyrene
Inchi:	InChI=1S/C16H10/c1-3-11-7-9-13-5-2-6-14-10-8-12(4-1)15(11)16(13)14/h1-10H
InchiKey:	BBEAQIROQSPTKN-UHFFFAOYSA-N
Formula:	C16H10
SMILES:	c1cc2ccc3cccc4ccc(c1)c2c34
Mol. weight [g/mol]:	202.25
CAS:	129-00-0

Physical Properties

Property code	Value	Unit	Source
affp	869.20	kJ/mol	NIST Webbook
affp	867.80	kJ/mol	NIST Webbook
basg	841.80	kJ/mol	NIST Webbook
basg	840.10	kJ/mol	NIST Webbook
chs	-7840.00 ± 3.50	kJ/mol	NIST Webbook
chs	-7850.70 ± 1.00	kJ/mol	NIST Webbook
chs	-7840.10 ± 0.40	kJ/mol	NIST Webbook
ea	0.39	eV	NIST Webbook
ea	0.59 ± 0.01	eV	NIST Webbook
ea	0.41 ± 0.01	eV	NIST Webbook
ea	0.50 ± 0.03	eV	NIST Webbook
gf	491.18	kJ/mol	Joback Method
hf	214.90	kJ/mol	NIST Webbook
hf	225.50 ± 2.50	kJ/mol	NIST Webbook
hf	225.70 ± 1.30	kJ/mol	NIST Webbook
hf	214.90	kJ/mol	NIST Webbook
hfs	114.70 ± 3.60	kJ/mol	NIST Webbook
hfs	125.20 ± 2.30	kJ/mol	NIST Webbook
hfs	114.70 ± 0.40	kJ/mol	NIST Webbook
hfs	125.50 ± 1.20	kJ/mol	NIST Webbook

h _{fus}	24.49	kJ/mol	Joback Method
h _{sub}	100.20	kJ/mol	NIST Webbook
h _{sub}	100.20 ± 0.40	kJ/mol	NIST Webbook
h _{sub}	100.30 ± 1.00	kJ/mol	NIST Webbook
h _{sub}	104.50	kJ/mol	NIST Webbook
h _{sub}	98.50 ± 1.00	kJ/mol	NIST Webbook
h _{vap}	92.40 ± 1.10	kJ/mol	NIST Webbook
h _{vap}	87.20 ± 1.30	kJ/mol	NIST Webbook
ie	7.48	eV	NIST Webbook
ie	7.40	eV	NIST Webbook
ie	7.70	eV	NIST Webbook
ie	7.41	eV	NIST Webbook
ie	7.41	eV	NIST Webbook
ie	7.43 ± 0.00	eV	NIST Webbook
ie	7.31	eV	NIST Webbook
ie	7.42	eV	NIST Webbook
ie	7.58	eV	NIST Webbook
ie	7.55	eV	NIST Webbook
ie	7.45 ± 0.01	eV	NIST Webbook
ie	7.72	eV	NIST Webbook
ie	7.41	eV	NIST Webbook
ie	7.50 ± 0.05	eV	NIST Webbook
ie	7.43 ± 0.00	eV	NIST Webbook
ie	7.45	eV	NIST Webbook
ie	7.53	eV	NIST Webbook
ie	7.70 ± 0.30	eV	NIST Webbook
log ₁₀ w _s	-6.18		Estimated Solubility Method
log ₁₀ w _s	-6.17		Aqueous Solubility Prediction Method
log _p	4.584		Crippen Method
m _{cvol}	158.460	ml/mol	McGowan Method
pc	2721.00	kPa	KDB
r _{inpol}	352.41		NIST Webbook
r _{inpol}	2104.00		NIST Webbook
r _{inpol}	2109.00		NIST Webbook
r _{inpol}	2109.00		NIST Webbook
r _{inpol}	2112.00		NIST Webbook
r _{inpol}	2114.00		NIST Webbook
r _{inpol}	2134.00		NIST Webbook
r _{inpol}	2135.00		NIST Webbook
r _{inpol}	2085.00		NIST Webbook
r _{inpol}	2096.00		NIST Webbook
r _{inpol}	2103.00		NIST Webbook
r _{inpol}	2114.00		NIST Webbook

rinpol	2077.00	NIST Webbook
rinpol	2103.00	NIST Webbook
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rinpol	351.74	NIST Webbook
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rinpol	2113.40	NIST Webbook
rinpol	2080.40	NIST Webbook
rinpol	2132.50	NIST Webbook
rinpol	2069.40	NIST Webbook
rinpol	2041.00	NIST Webbook
rinpol	2055.00	NIST Webbook
rinpol	2078.00	NIST Webbook
rinpol	2093.00	NIST Webbook
rinpol	348.91	NIST Webbook
rinpol	351.74	NIST Webbook
rinpol	2089.00	NIST Webbook
rinpol	2044.00	NIST Webbook
rinpol	2136.00	NIST Webbook
rinpol	2120.64	NIST Webbook
rinpol	2069.70	NIST Webbook
rinpol	2040.00	NIST Webbook
rinpol	2070.00	NIST Webbook
rinpol	2048.56	NIST Webbook

rinpol	2063.99	NIST Webbook
rinpol	2093.00	NIST Webbook
rinpol	2086.00	NIST Webbook
rinpol	2086.00	NIST Webbook
rinpol	2080.00	NIST Webbook
rinpol	2079.00	NIST Webbook
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rinpol	2041.00	NIST Webbook
rinpol	2057.00	NIST Webbook
rinpol	2073.47	NIST Webbook
rinpol	2091.45	NIST Webbook
rinpol	2069.26	NIST Webbook
rinpol	2069.40	NIST Webbook
rinpol	2060.85	NIST Webbook
rinpol	2049.68	NIST Webbook
rinpol	2113.40	NIST Webbook
rinpol	2113.40	NIST Webbook
rinpol	2132.50	NIST Webbook
rinpol	2113.40	NIST Webbook
rinpol	2082.60	NIST Webbook
rinpol	2095.80	NIST Webbook
rinpol	2126.40	NIST Webbook
rinpol	2080.40	NIST Webbook
rinpol	2132.50	NIST Webbook
rinpol	2113.40	NIST Webbook
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rinpol	2101.00	NIST Webbook
rinpol	2119.00	NIST Webbook
rinpol	2103.00	NIST Webbook
rinpol	2055.00	NIST Webbook
rinpol	351.22	NIST Webbook
rinpol	2046.00	NIST Webbook
ripol	3183.00	NIST Webbook
ripol	3135.00	NIST Webbook

ripol	3183.00		NIST Webbook
ripol	3160.00		NIST Webbook
ripol	3160.00		NIST Webbook
ss	224.89	J/molxK	NIST Webbook
ss	215.10	J/molxK	NIST Webbook
tb	666.00	K	KDB
tc	938.20	K	KDB
tc	974.00	K	Critical point measurement of some polycyclic aromatic hydrocarbons
tf	423.90	K	Isothermal Thermogravimetric Study for Determining Sublimation Enthalpies of Some Hydroxyflavones
tf	427.00 ± 2.00	K	NIST Webbook
tf	421.25 ± 1.00	K	NIST Webbook
tf	425.40 ± 0.30	K	NIST Webbook
tf	424.30 ± 0.60	K	NIST Webbook
tf	424.15 ± 1.50	K	NIST Webbook
tf	423.90	K	Experimental and computational thermodynamics of pyrene and 1-pyrenecarboxaldehyde and their photophysical properties
tf	425.83	K	Aqueous Solubility Prediction Method
tf	423.80	K	KDB
tf	425.70 ± 1.00	K	NIST Webbook
tf	423.60 ± 0.30	K	NIST Webbook
tf	424.50 ± 0.10	K	NIST Webbook
tt	423.81 ± 0.01	K	NIST Webbook
vc	0.626	m ³ /kmol	KDB
zc	0.2183590		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.86	J/molxK	822.10	Joback Method
cpg	400.96	J/molxK	694.05	Joback Method
cpg	454.56	J/molxK	907.48	Joback Method
cpg	444.86	J/molxK	864.79	Joback Method
cpg	387.64	J/molxK	651.36	Joback Method
cpg	413.12	J/molxK	736.73	Joback Method

cpg	424.36	J/molxK	779.42	Joback Method
cps	227.65	J/molxK	291.10	NIST Webbook
cps	229.70	J/molxK	298.15	NIST Webbook
cps	229.36	J/molxK	298.15	NIST Webbook
dvisc	0.0013128	Paxs	651.36	Joback Method
dvisc	0.0018191	Paxs	463.49	Joback Method
dvisc	0.0014580	Paxs	576.21	Joback Method
dvisc	0.0015536	Paxs	538.64	Joback Method
dvisc	0.0020100	Paxs	425.92	Joback Method
dvisc	0.0013791	Paxs	613.79	Joback Method
dvisc	0.0016712	Paxs	501.07	Joback Method
hfust	17.36	kJ/mol	423.80	NIST Webbook
hfust	0.29	kJ/mol	120.80	NIST Webbook
hfust	17.36	kJ/mol	423.80	NIST Webbook
hfust	16.70	kJ/mol	418.00	NIST Webbook
hsubt	100.30 ± 0.30	kJ/mol	376.00	NIST Webbook
hsubt	100.80 ± 1.50	kJ/mol	383.50	NIST Webbook
hsubt	91.20 ± 0.50	kJ/mol	303.00	NIST Webbook
hsubt	100.20 ± 0.40	kJ/mol	410.50	NIST Webbook
hsubt	103.30 ± 2.10	kJ/mol	379.50	NIST Webbook
hsubt	103.10 ± 6.50	kJ/mol	353.00	NIST Webbook
hsubt	100.10 ± 1.70	kJ/mol	351.50	NIST Webbook
hsubt	94.14	kJ/mol	344.75	NIST Webbook
hsubt	100.50	kJ/mol	330.50	NIST Webbook
hsubt	97.90	kJ/mol	383.00	NIST Webbook
hvapt	76.40	kJ/mol	428.00	NIST Webbook
hvapt	73.00	kJ/mol	590.50	NIST Webbook
hvapt	76.00	kJ/mol	440.00	NIST Webbook
hvapt	78.60	kJ/mol	398.00	NIST Webbook
hvapt	81.50	kJ/mol	435.00	Evaluation of sublimation enthalpy by thermogravimetry: Analysis of the diffusion effects in the case of methyl and phenyl substituted hydantoins
psub	1.71e-04	kPa	351.05	Thermal Stability, Sublimation Pressures, and Diffusion Coefficients of Anthracene, Pyrene, and Some Metal beta-Diketonates

psub	0.01	kPa	398.55	Thermal Stability, Sublimation Pressures, and Diffusion Coefficients of Anthracene, Pyrene, and Some Metal beta-Diketonates
psub	0.03	kPa	408.05	Thermal Stability, Sublimation Pressures, and Diffusion Coefficients of Anthracene, Pyrene, and Some Metal beta-Diketonates
psub	0.02	kPa	402.05	Thermal Stability, Sublimation Pressures, and Diffusion Coefficients of Anthracene, Pyrene, and Some Metal beta-Diketonates
psub	8.46e-03	kPa	392.95	Thermal Stability, Sublimation Pressures, and Diffusion Coefficients of Anthracene, Pyrene, and Some Metal beta-Diketonates
psub	5.39e-03	kPa	389.05	Thermal Stability, Sublimation Pressures, and Diffusion Coefficients of Anthracene, Pyrene, and Some Metal beta-Diketonates
psub	4.72e-03	kPa	383.95	Thermal Stability, Sublimation Pressures, and Diffusion Coefficients of Anthracene, Pyrene, and Some Metal beta-Diketonates
psub	1.97e-03	kPa	379.55	Thermal Stability, Sublimation Pressures, and Diffusion Coefficients of Anthracene, Pyrene, and Some Metal beta-Diketonates

psub	1.47e-03	kPa	373.95	Thermal Stability, Sublimation Pressures, and Diffusion Coefficients of Anthracene, Pyrene, and Some Metal beta-Diketonates
psub	8.82e-04	kPa	369.85	Thermal Stability, Sublimation Pressures, and Diffusion Coefficients of Anthracene, Pyrene, and Some Metal beta-Diketonates
psub	7.50e-05	kPa	341.45	Thermal Stability, Sublimation Pressures, and Diffusion Coefficients of Anthracene, Pyrene, and Some Metal beta-Diketonates
psub	2.81e-03	kPa	381.40	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	1.30e-03	kPa	372.00	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	5.99e-04	kPa	362.10	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	3.39e-04	kPa	356.80	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method

psub	2.27e-04	kPa	352.30	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	1.47e-04	kPa	347.10	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	9.43e-05	kPa	342.10	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	5.31e-05	kPa	337.10	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	8.95e-06	kPa	322.00	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	8.27e-04	kPa	363.63	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures
psub	1.21e-04	kPa	343.36	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures

psub	4.56e-05	kPa	333.53	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures
psub	1.41e-05	kPa	323.81	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures
psub	3.64e-06	kPa	313.61	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures
psub	3.29e-04	kPa	353.24	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures
pvap	1.05	kPa	480.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.49	kPa	490.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.08	kPa	500.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	2.84	kPa	510.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.72	kPa	470.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.49	kPa	460.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.32	kPa	450.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.21	kPa	440.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.13	kPa	430.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.08	kPa	420.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	0.04	kPa	410.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.03	kPa	400.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.01	kPa	390.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.97e-03	kPa	380.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.43e-03	kPa	370.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.60e-03	kPa	360.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	7.06e-04	kPa	350.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	2.92e-04	kPa	340.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.13e-04	kPa	330.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.06e-05	kPa	320.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.34e-05	kPa	310.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.22e-06	kPa	298.15	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.07e-06	kPa	300.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
rho1	1274.21	kg/m3	293.10	KDB
sfust	40.97	J/molxK	423.80	NIST Webbook
sfust	2.39	J/molxK	120.80	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.50707e+01
Coeff. B	-6.21237e+03
Coeff. C	-7.35980e+01
Temperature range (K), min.	493.83
Temperature range (K), max.	710.16

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	8.81031e+01
Coeff. B	-1.32178e+04
Coeff. C	-9.93042e+00
Coeff. D	2.04131e-06
Temperature range (K), min.	423.81
Temperature range (K), max.	936.00

Sources

Thermal Stability, Sublimation Pressures, and Diffusion Coefficients of Polychlorinated Biphenyls and Polycyclic Aromatic Hydrocarbons in Air and Water: A Review
<https://www.doi.org/10.1021/je9001653>

Solubility of Pyrene, and Some Metal Ions, Dissolved in Alcohol + Acetone Mixtures Method
<https://www.doi.org/10.1021/je020226c>

Experimental and computational thermodynamics of pyrene and perylene in the air/water and water/microemulsion systems
http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Partition Coefficients and Henry's Law Constants of Polychlorinated Biphenyls and Polycyclic Aromatic Hydrocarbons in Water and Pyrene dissolved in alcohol + toluene aqueous solutions
<https://www.doi.org/10.1016/j.jct.2015.07.008>

Determination of Henry's Law Constant Using Diffusion in Air and Water Boundary Layers
<https://www.doi.org/10.1021/je900967j>

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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
pvap:	Vapor pressure
rho:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

sfust:	Entropy of fusion at a given temperature
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
zc:	Critical Compressibility

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