Fluoranthene

Other names:	1,2-(1,8-NAPHTHYLENE)-BENZENE
	1,2-(1,8-Naphthalene)benzene
	1,2-(1,8-Naphthalenediyl)benzene
	1,2-(1,8-Naphthylene)benzene
	1,2-Benzacenaphthene
	Benzene, 1,2-(1,8-naphthalenediyl)-
	Benzene, 1,2-(1,8-naphthylene)-
	Benzo[jk]fluorene
	Fluoranthrene
	Idryl
	NSC 6803
	Rcra waste number U120
Inchi:	InChI=1S/C16H10/c1-2-8-13-12(7-1)14-9-3-5-11-6-4-10-15(13)16(11)14/h1-10H
InchiKey:	GVEPBJHOBDJJJI-UHFFFAOYSA-N
Formula:	C16H10
SMILES:	c1ccc2c(c1)-c1cccc3cccc-2c13
Mol. weight [g/mol]:	202.25
CAS:	206-44-0

Physical Properties

Property code	Value	Unit	Source
affp	828.60	kJ/mol	NIST Webbook
affp	826.80	kJ/mol	NIST Webbook
basg	799.60	kJ/mol	NIST Webbook
basg	800.90	kJ/mol	NIST Webbook
chs	-7917.80 ± 5.40	kJ/mol	NIST Webbook
chs	-7915.20 ± 0.40	kJ/mol	NIST Webbook
ea	0.63	eV	NIST Webbook
gf	491.18	kJ/mol	Joback Method
hf	289.80	kJ/mol	NIST Webbook
hf	292.00 ± 2.20	kJ/mol	NIST Webbook
hf	291.40 ± 4.00	kJ/mol	NIST Webbook
hfs	192.00 ± 5.40	kJ/mol	NIST Webbook
hfs	189.80 ± 0.40	kJ/mol	NIST Webbook
hfs	190.20 ± 2.80	kJ/mol	NIST Webbook
hfus	24.49	kJ/mol	Joback Method
hsub	99.20 ± 0.80	kJ/mol	NIST Webbook

hsub	101.20 ± 2.80	kJ/mol	NIST Webbook
hsub	102.00 ± 2.00	kJ/mol	NIST Webbook
hsub	99.20 ± 0.80	kJ/mol	NIST Webbook
hsub	100.00	kJ/mol	NIST Webbook
hvap	86.80 ± 1.30	kJ/mol	NIST Webbook
ie	7.80 ± 0.01	eV	NIST Webbook
ie	7.90 ± 0.10	eV	NIST Webbook
ie	7.95 ± 0.04	eV	NIST Webbook
ie	7.90 ± 0.10	eV	NIST Webbook
ie	7.72	eV	NIST Webbook
log10ws	-6.00		Estimated Solubility Method
log10ws	-5.95		Aqueous Solubility Prediction Method
logp	4.487		Crippen Method
mcvol	158.460	ml/mol	McGowan Method
pc	3072.75	kPa	Joback Method
rinpol	2009.00		NIST Webbook
rinpol	2023.00		NIST Webbook
rinpol	2030.00		NIST Webbook
rinpol	2030.00		NIST Webbook
rinpol	2031.00		NIST Webbook
rinpol	2037.00		NIST Webbook
rinpol	2042.00		NIST Webbook
rinpol	2044.00		NIST Webbook
rinpol	2020.00		NIST Webbook
rinpol	2020.45		NIST Webbook
rinpol	2068.42		NIST Webbook
rinpol	2084.00		NIST Webbook
rinpol	2037.00		NIST Webbook
rinpol	2015.00		NIST Webbook
rinpol	2098.00		NIST Webbook
rinpol	2089.00		NIST Webbook
rinpol	2052.00		NIST Webbook
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rinpol	2058.00		NIST Webbook
rinpol	2060.00		NIST Webbook
rinpol	2061.00		NIST Webbook
rinpol	2079.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2031.00		NIST Webbook
rinpol	2045.00		NIST Webbook
rinpol	2062.00		NIST Webbook
rinpol	2028.00		NIST Webbook

rinpol	2006.00	NIST Webbook
rinpol	2084.00	NIST Webbook
rinpol	2085.00	NIST Webbook
rinpol	2030.00	NIST Webbook
rinpol	2091.00	NIST Webbook
rinpol	341.94	NIST Webbook
rinpol	340.99	NIST Webbook
rinpol	343.44	NIST Webbook
rinpol	343.15	NIST Webbook
rinpol	342.27	NIST Webbook
rinpol	343.16	NIST Webbook
rinpol	344.01	NIST Webbook
rinpol	344.30	NIST Webbook
rinpol	337.00	NIST Webbook
rinpol	337.00	NIST Webbook
rinpol	344.01	NIST Webbook
rinpol	340.90	NIST Webbook
rinpol	344.85	NIST Webbook
rinpol	344.49	NIST Webbook
rinpol	344.78	NIST Webbook
rinpol	344.83	NIST Webbook
rinpol	344.99	NIST Webbook
rinpol	344.49	NIST Webbook
rinpol	344.51	NIST Webbook
rinpol	344.56	NIST Webbook
rinpol	344.60	NIST Webbook
rinpol	344.64	NIST Webbook
rinpol	344.67	NIST Webbook
rinpol	344.74	NIST Webbook
rinpol	344.75	NIST Webbook
rinpol	344.54	NIST Webbook
rinpol	344.68	NIST Webbook
rinpol	344.80	NIST Webbook
rinpol	344.80	NIST Webbook
rinpol	344.67	NIST Webbook
rinpol	344.85	NIST Webbook
rinpol	344.80	NIST Webbook
rinpol	345.00	NIST Webbook
rinpol	344.55	NIST Webbook
rinpol	344.62	NIST Webbook
rinpol	2023.00	NIST Webbook
rinpol	344.49	NIST Webbook
rinpol	344.68	NIST Webbook
rinpol	344.43	NIST Webbook

rinpol	340.66	NIST Webbook
rinpol	344.56	NIST Webbook
rinpol	344.70	NIST Webbook
rinpol	344.51	NIST Webbook
rinpol	344.01	NIST Webbook
rinpol	344.60	NIST Webbook
rinpol	344.96	NIST Webbook
rinpol	344.49	NIST Webbook
rinpol	344.96	NIST Webbook
rinpol	340.10	NIST Webbook
rinpol	338.20	NIST Webbook
rinpol	389.98	NIST Webbook
rinpol	340.21	NIST Webbook
rinpol	340.44	NIST Webbook
rinpol	338.50	NIST Webbook
rinpol	344.00	NIST Webbook
rinpol	344.90	NIST Webbook
rinpol	340.35	NIST Webbook
rinpol	340.44	NIST Webbook
rinpol	342.65	NIST Webbook
rinpol	343.25	NIST Webbook
rinpol	343.31	NIST Webbook
rinpol	344.01	NIST Webbook
rinpol	344.51	NIST Webbook
rinpol	343.24	NIST Webbook
rinpol	344.60	NIST Webbook
rinpol	340.11	NIST Webbook
rinpol	344.01	NIST Webbook
rinpol	345.32	NIST Webbook
rinpol	344.60	NIST Webbook
rinpol	340.05	NIST Webbook
rinpol	340.88	NIST Webbook
rinpol	341.74	NIST Webbook
rinpol	342.74	NIST Webbook
rinpol	343.25	NIST Webbook
rinpol	343.65	NIST Webbook
rinpol	344.01	NIST Webbook
rinpol	345.00	NIST Webbook
rinpol	341.94	NIST Webbook
rinpol	343.16	NIST Webbook
rinpol	2098.00	NIST Webbook
rinpol	2058.00	NIST Webbook
rinpol	2031.00	NIST Webbook
rinpol	344.30	NIST Webbook

rinpol	344.85		NIST Webbook
rinpol	344.49		NIST Webbook
rinpol	2023.00		NIST Webbook
rinpol	344.80		NIST Webbook
rinpol	345.00		NIST Webbook
rinpol	344.68		NIST Webbook
rinpol	344.51		NIST Webbook
rinpol	2062.00		NIST Webbook
rinpol	2030.00		NIST Webbook
rinpol	2020.45		NIST Webbook
rinpol	2023.00		NIST Webbook
rinpol	2009.00		NIST Webbook
rinpol	2009.00		NIST Webbook
rinpol	2009.00		NIST Webbook
rinpol	2009.00		NIST Webbook
rinpol	2011.00		NIST Webbook
rinpol	2084.00		NIST Webbook
rinpol	2060.10		NIST Webbook
rinpol	2060.10		NIST Webbook
rinpol	2076.50		NIST Webbook
rinpol	2060.10		NIST Webbook
rinpol	2032.60		NIST Webbook
rinpol	2085.00		NIST Webbook
rinpol	2062.30		NIST Webbook
rinpol	2038.90		NIST Webbook
rinpol	2076.50		NIST Webbook
rinpol	2060.10		NIST Webbook
rinpol	2032.60		NIST Webbook
rinpol	2060.10		NIST Webbook
rinpol	2060.10		NIST Webbook
rinpol	2053.50		NIST Webbook
rinpol	2091.00		NIST Webbook
rinpol	2051.00		NIST Webbook
rinpol	2091.00		NIST Webbook
rinpol	2091.00		NIST Webbook
rinpol	2057.00		NIST Webbook
rinpol	344.35		NIST Webbook
rinpol	344.67		NIST Webbook
ss	230.58	J/mol×K	NIST Webbook
tb	651.36	K	Joback Method
tc	907.48	K	Joback Method
tf	383.45 ± 1.00	K	NIST Webbook
tf	381.00 ± 0.20	K	NIST Webbook

tf	381.50	K	Polar Mixed-Solid Solute Systems in Supercritical Carbon Dioxide: Entrainer Effect and Its Influence on Solubility and Selectivity
tf	386.10 ± 3.00	K	NIST Webbook
tf	381.10	K	Aqueous Solubility Prediction Method
tf	385.40 ± 3.00	K	NIST Webbook
tf	385.20 ± 3.00	K	NIST Webbook
tt	383.33 ± 0.01	K	NIST Webbook
tt	383.34 ± 0.01	K	NIST Webbook
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.56	J/mol×K	907.48	Joback Method
cpg	424.36	J/mol×K	779.42	Joback Method
cpg	434.86	J/mol×K	822.10	Joback Method
cpg	444.86	J/mol×K	864.79	Joback Method
cpg	400.96	J/mol×K	694.05	Joback Method
cpg	387.64	J/mol×K	651.36	Joback Method
cpg	413.12	J/mol×K	736.73	Joback Method
cps	230.25	J/mol×K	298.15	NIST Webbook
dvisc	0.0015536	Pa×s	538.64	Joback Method
dvisc	0.0013128	Pa×s	651.36	Joback Method
dvisc	0.0013791	Pa×s	613.79	Joback Method
dvisc	0.0014580	Pa×s	576.21	Joback Method
dvisc	0.0016712	Pa×s	501.07	Joback Method
dvisc	0.0018191	Pa×s	463.49	Joback Method
dvisc	0.0020100	Pa×s	425.92	Joback Method
hfust	18.73	kJ/mol	383.36	NIST Webbook
hfust	18.74	kJ/mol	383.40	NIST Webbook
hsubt	102.60	kJ/mol	328.00	NIST Webbook
hsubt	102.00 ± 2.00	kJ/mol	340.50	NIST Webbook
hsubt	84.60 ± 0.90	kJ/mol	303.00	NIST Webbook
hsubt	98.30	kJ/mol	383.00	NIST Webbook
hvapt	79.30	kJ/mol	398.00	NIST Webbook
hvapt	62.20	kJ/mol	580.50	NIST Webbook
hvapt	77.40	kJ/mol	398.00	NIST Webbook

psub	2.06e-04	kPa	342.50	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	1.05e-03	kPa	359.20	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	4.63e-04	kPa	350.90	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	5.80e-04	kPa	354.10	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	3.41e-04	kPa	348.50	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	3.30e-04	kPa	348.00	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	2.58e-04	kPa	345.30	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method

psub	2.48e-04	kPa	343.90	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	1.54e-04	kPa	340.20	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	1.44e-04	kPa	338.90	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	1.31e-04	kPa	338.80	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	1.29e-04	kPa	338.70	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	1.17e-04	kPa	336.70	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	
psub	6.32e-05	kPa	331.80	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	

psub	6.16e-05	kPa	331.00	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	4.11e-05	kPa	326.90	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	3.96e-05	kPa	326.80	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
sfust	48.85	J/mol×K	383.36	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59674e+01
Coeff. B	-7.14694e+03
Coeff. C	-2.76650e+01
Temperature range (K), min.	483.47
Temperature range (K), max.	698.36

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.00473e+02
Coeff. B	-1.29109e+04
Coeff. C	-1.20342e+01
Coeff. D	4.37832e-06
Temperature range (K), min.	383.15

Temperature range (K), max.	905.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C206440&Units=SI
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=799
Determination of Henry's Law Constant Using Diffusion in Air and Water Boundary Layers:	https://www.doi.org/10.1021/je300954s
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Polar Mixed-Solid Solute Systems in Supercritical Carbon Dioxide: Entrainer Effect and Its Influence on Solubility	https://www.doi.org/10.1021/je700486g
Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method:	https://www.doi.org/10.1021/je7005133
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=799
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
rinpol:	Non-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