Acenaphthene

Other names:	1,2-DIHYDRO-ACENAPHTHYLENE 1,2-Dihydroacenaphthylene 1,8-Ethylenenaphthalene Acenaphthylene, 1,2-dihydro- Naphthyleneethylene Peri-Ethylenenaphthalene acenaphtene
Inchi:	InChI=1S/C12H10/c1-3-9-4-2-6-11-8-7-10(5-1)12(9)11/h1-6H,7-8H2
InchiKey:	CWRYPZZKDGJXCA-UHFFFAOYSA-N
Formula:	C12H10
SMILES:	c1cc2c3c(cccc3c1)CC2
Mol. weight [g/mol]:	154.21
CAS:	83-32-9

Physical Properties

Property code	Value	Unit	Source
affp	851.70	kJ/mol	NIST Webbook
affp	849.80	kJ/mol	NIST Webbook
basg	821.70	kJ/mol	NIST Webbook
basg	821.00	kJ/mol	NIST Webbook
chs	-6222.00 ± 3.00	kJ/mol	NIST Webbook
gf	330.52	kJ/mol	Joback Method
hf	156.00 ± 4.00	kJ/mol	NIST Webbook
hf	156.80 ± 3.10	kJ/mol	NIST Webbook
hfs	70.00 ± 3.00	kJ/mol	NIST Webbook
hfs	72.00 ± 3.10	kJ/mol	NIST Webbook
hfus	16.28	kJ/mol	Joback Method
hsub	86.00	kJ/mol	NIST Webbook
hsub	86.00 ± 1.00	kJ/mol	NIST Webbook
hsub	83.40 ± 1.00	kJ/mol	NIST Webbook
hsub	84.80 ± 0.40	kJ/mol	NIST Webbook
hsub	84.60	kJ/mol	NIST Webbook
hvap	70.50 ± 1.10	kJ/mol	NIST Webbook
hvap	66.20	kJ/mol	NIST Webbook
hvap	66.50 ± 1.30	kJ/mol	NIST Webbook
hvap	66.20	kJ/mol	NIST Webbook
hvap	68.00	kJ/mol	NIST Webbook

ie	7.66	eV	NIST Webbook
ie	7.82 ± 0.04	eV	NIST Webbook
ie	7.68 ± 0.05	eV	NIST Webbook
ie	7.73 ± 0.01	eV	NIST Webbook
ie	7.76 ± 0.03	eV	NIST Webbook
ie	7.75 ± 0.05	eV	NIST Webbook
log10ws	-4.58		Aqueous Solubility Prediction Method
logp	2.938		Crippen Method
mcvol	125.860	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
rinpol	1491.00		NIST Webbook
rinpol	1481.40		NIST Webbook
rinpol	1480.50		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1481.40		NIST Webbook
rinpol	1488.60		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1481.40		NIST Webbook
rinpol	1488.60		NIST Webbook
rinpol	1481.40		NIST Webbook
rinpol	1480.50		NIST Webbook
rinpol	1445.50		NIST Webbook
rinpol	1445.30		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1481.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1455.06		NIST Webbook
rinpol	1488.20		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1439.00		NIST Webbook
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rinpol	1450.00		NIST Webbook
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rinpol	1455.00		NIST Webbook
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rinpol	1503.00	NIST Webbook
rinpol	1492.00	NIST Webbook
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rinpol	1457.00	NIST Webbook
rinpol	1476.00	NIST Webbook
rinpol	1447.00	NIST Webbook
rinpol	1446.00	NIST Webbook
rinpol	1463.90	NIST Webbook
rinpol	1494.00	NIST Webbook
rinpol	1494.00	NIST Webbook
rinpol	1522.00	NIST Webbook
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rinpol	242.90	NIST Webbook
rinpol	243.10	NIST Webbook
rinpol	251.29	NIST Webbook
rinpol	253.30	NIST Webbook
rinpol	254.07	NIST Webbook
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rinpol	254.87	NIST Webbook
rinpol	254.36	NIST Webbook
rinpol	254.04	NIST Webbook
rinpol	254.10	NIST Webbook
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rinpol	254.30	NIST Webbook

rinpol	254.33	NIST Webbook
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rinpol	254.98	NIST Webbook
rinpol	231.65	NIST Webbook
rinpol	253.14	NIST Webbook
rinpol	251.29	NIST Webbook
rinpol	255.00	NIST Webbook
rinpol	253.56	NIST Webbook
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rinpol	253.67	NIST Webbook
rinpol	254.50	NIST Webbook
rinpol	251.99	NIST Webbook
rinpol	245.85	NIST Webbook
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rinpol	1475.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	254.04		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1485.00		NIST Webbook
ripol	2092.00		NIST Webbook
ripol	2132.00		NIST Webbook
ripol	2108.00		NIST Webbook
ripol	2133.00		NIST Webbook
ripol	2103.00		NIST Webbook
ss	188.87	J/mol×K	NIST Webbook
tb	502.65 ± 1.00	K	NIST Webbook
tb	552.00	K	NIST Webbook
tb	552.20	K	NIST Webbook
tc	820.00	K	Critical point measurement of some polycyclic aromatic hydrocarbons
tf	367.55	K	Aqueous Solubility Prediction Method
tt	366.56 ± 0.02	K	NIST Webbook
tt	366.55 ± 0.02	K	NIST Webbook
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.39	J/mol×K	777.86	Joback Method
cpg	294.23	J/mol×K	576.91	Joback Method
cpg	307.22	J/mol×K	617.10	Joback Method
cpg	319.10	J/mol×K	657.29	Joback Method
cpg	329.99	J/mol×K	697.48	Joback Method
cpg	340.05	J/mol×K	737.67	Joback Method

cpg	280.00	J/mol×K	536.72	Joback Method
cps	210.50	J/mol×K	298.10	NIST Webbook
cps	190.37	J/mol×K	298.15	NIST Webbook
cps	185.80	J/mol×K	298.00	NIST Webbook
dvisc	0.0007316	Pa×s	536.72	Joback Method
dvisc	0.0010583	Pa×s	402.15	Joback Method
dvisc	0.0012105	Pa×s	368.50	Joback Method
dvisc	0.0014227	Pa×s	334.86	Joback Method
dvisc	0.0008569	Pa×s	469.43	Joback Method
dvisc	0.0007876	Pa×s	503.08	Joback Method
dvisc	0.0009445	Pa×s	435.79	Joback Method
hfust	25.10	kJ/mol	367.80	NIST Webbook
hfust	21.46	kJ/mol	366.60	NIST Webbook
hfust	21.46	kJ/mol	366.60	NIST Webbook
hfust	21.00	kJ/mol	367.00	NIST Webbook
hfust	21.46	kJ/mol	366.56	NIST Webbook
hfust	20.23	kJ/mol	366.40	NIST Webbook
hsubt	77.00	kJ/mol	317.50	NIST Webbook
hsubt	81.60	kJ/mol	283.00	NIST Webbook
hsubt	86.80 ± 0.90	kJ/mol	303.00	NIST Webbook
hsubt	83.20	kJ/mol	383.00	NIST Webbook
hsubt	82.40	kJ/mol	366.00	NIST Webbook
hsubt	82.13 ± 0.42	kJ/mol	368.00	NIST Webbook
hsubt	84.70 ± 2.70	kJ/mol	283.00	NIST Webbook
hsubt	86.20 ± 0.80	kJ/mol	315.00	NIST Webbook
hsubt	82.10 ± 0.40	kJ/mol	300.50	NIST Webbook
hvapt	61.30	kJ/mol	395.00	NIST Webbook
hvapt	55.40	kJ/mol	490.50	NIST Webbook
hvapt	54.30	kJ/mol	487.00	NIST Webbook
hvapt	60.30	kJ/mol	390.50	NIST Webbook
hvapt	54.00	kJ/mol	460.00	NIST Webbook
hvapt	61.10	kJ/mol	366.00	NIST Webbook
hvapt	67.98	kJ/mol	298.00	Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons. Liquid-Vapor Pressure Isotope Effects
hvapt	60.60	kJ/mol	378.00	NIST Webbook
hvapt	63.90	kJ/mol	398.00	NIST Webbook

psub	1.80e-03	kPa	315.60	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	4.40e-04	kPa	301.60	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	4.13e-04	kPa	300.50	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	3.62e-04	kPa	299.70	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	1.12e-03	kPa	310.70	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	6.93e-04	kPa	306.10	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	5.08e-04	kPa	302.80	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method

psub	2.90e-04	kPa	297.60	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
sfust	58.55	J/mol×K	366.56	NIST Webbook
sfust	55.22	J/mol×K	366.40	NIST Webbook
sfust	68.20	J/mol×K	367.80	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.24317e+01
Coeff. B	-7.30879e+03
Coeff. C	-7.54360e+01
Temperature range (K), min.	405.49
Temperature range (K), max.	502.35

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.77558e+01
Coeff. B	-9.75784e+03
Coeff. C	-7.27940e+00
Coeff. D	1.74725e-06
Temperature range (K), min.	366.15
Temperature range (K), max.	803.15

Sources

Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method	https://www.doi.org/10.1021/je7005133
Solubility of Acenaphthene in Different Solvents from (293.00 to 323.00) K:	https://www.doi.org/10.1021/je8006869
Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons: Liquid-Vapor Pressure Isotope Effects:	https://www.doi.org/10.1021/je800091s
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C83329&Units=SI

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=766
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
Determination of Henry's Law Constant Using Diffusion in Air and Water Boundary Layers:	https://www.doi.org/10.1021/je300954s
Critical point measurement of some polycyclic aromatic hydrocarbons:	https://www.doi.org/10.1016/j.jct.2014.09.004
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=766
Solid-liquid phase equilibrium of 9-fluorenone and several polynuclear aromatic hydrocarbons:	https://www.doi.org/10.1016/j.fluid.2012.01.017
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=766
Solid Liquid Phase Equilibrium and Solubility of Dibenzo[b,d]furan and 9H-Fluoren-9-one in Organic Solvents:	https://www.doi.org/10.1021/je201282d
Solubility of Acenaphthene, Anthracene, and Pyrene in Water At 50 to 80 °C:	https://www.doi.org/10.1021/je0495886
Solid-liquid equilibrium of some polycyclic aromatic hydrocarbons in Washoil:	https://www.doi.org/10.1016/j.fluid.2012.01.031
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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
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

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