Acenaphthylene

Other names:	Acenaphthalene
	Acenapthylene
	Cyclopenta[de]naphthalene
Inchi:	InChI=1S/C12H8/c1-3-9-4-2-6-11-8-7-10(5-1)12(9)11/h1-8H
InchiKey:	HXGDTGSAIMULJN-UHFFFAOYSA-N
Formula:	C12H8
SMILES:	C1=Cc2cccc3cccc1c23
Mol. weight [g/mol]:	152.19
CAS:	208-96-8

Physical Properties

Property code	Value	Unit	Source
affp	861.10	kJ/mol	NIST Webbook
basg	832.60	kJ/mol	NIST Webbook
chs	-6052.20 ± 4.60	kJ/mol	NIST Webbook
chs	-6058.00 ± 4.00	kJ/mol	NIST Webbook
ea	0.40 ± 0.03	eV	NIST Webbook
gf	360.48	kJ/mol	Joback Method
hf	264.00	kJ/mol	NIST Webbook
hf	263.20 ± 3.70	kJ/mol	NIST Webbook
hf	258.00 ± 5.90	kJ/mol	NIST Webbook
hfs	187.00 ± 4.60	kJ/mol	NIST Webbook
hfs	193.00 ± 4.00	kJ/mol	NIST Webbook
hfs	190.80 ± 3.50	kJ/mol	NIST Webbook
hfus	11.73	kJ/mol	Recommended vapor pressures for acenaphthylene, fluoranthene, and fluorene
hsub	70.00	kJ/mol	NIST Webbook
hsub	73.00 ± 0.30	kJ/mol	NIST Webbook
hsub	73.00 ± 0.40	kJ/mol	NIST Webbook
hsub	71.00 ± 1.00	kJ/mol	NIST Webbook
hsub	71.00	kJ/mol	NIST Webbook
hsub	72.50 ± 1.20	kJ/mol	NIST Webbook
hvap	69.10 ± 2.20	kJ/mol	NIST Webbook
hvap	64.60 ± 5.80	kJ/mol	NIST Webbook
ie	8.22 ± 0.04	eV	NIST Webbook
ie	8.02 ± 0.01	eV	NIST Webbook

ie	8.12 ± 0.10	eV	NIST Webbook
log10ws	-3.96		Aqueous Solubility Prediction Method
log10ws	-3.96		Estimated Solubility Method
logp	3.324		Crippen Method
mcvol	121.560	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
rinpol	1409.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1408.90		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1425.03		NIST Webbook
rinpol	1413.00		NIST Webbook
rinpol	1418.54		NIST Webbook
rinpol	1453.37		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1454.00		NIST Webbook
rinpol	1450.70		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1422.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1403.00		NIST Webbook
rinpol	1438.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1466.00		NIST Webbook
rinpol	1433.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	247.80		NIST Webbook
rinpol	244.63		NIST Webbook
rinpol	247.40		NIST Webbook
rinpol	248.47		NIST Webbook
rinpol	248.88		NIST Webbook
rinpol	248.48		NIST Webbook
rinpol	248.29		NIST Webbook
rinpol	247.93		NIST Webbook

rinpol	1457.55	NIST Webbook
rinpol	245.40	NIST Webbook
rinpol	249.00	NIST Webbook
rinpol	249.04	NIST Webbook
rinpol	245.83	NIST Webbook
rinpol	245.36	NIST Webbook
rinpol	249.19	NIST Webbook
rinpol	248.90	NIST Webbook
rinpol	247.82	NIST Webbook
rinpol	244.79	NIST Webbook
rinpol	247.65	NIST Webbook
rinpol	244.63	NIST Webbook
rinpol	248.75	NIST Webbook
rinpol	243.59	NIST Webbook
rinpol	242.46	NIST Webbook
rinpol	246.92	NIST Webbook
rinpol	244.63	NIST Webbook
rinpol	249.20	NIST Webbook
rinpol	248.27	NIST Webbook
rinpol	247.65	NIST Webbook
rinpol	248.27	NIST Webbook
rinpol	249.20	NIST Webbook
rinpol	240.45	NIST Webbook
rinpol	240.53	NIST Webbook
rinpol	244.60	NIST Webbook
rinpol	247.40	NIST Webbook
rinpol	247.70	NIST Webbook
rinpol	247.40	NIST Webbook
rinpol	240.52	NIST Webbook
rinpol	240.53	NIST Webbook
rinpol	244.63	NIST Webbook
rinpol	244.63	NIST Webbook
rinpol	253.15	NIST Webbook
rinpol	249.50	NIST Webbook
rinpol	244.00	NIST Webbook
rinpol	244.63	NIST Webbook
rinpol	247.80	NIST Webbook
rinpol	248.48	NIST Webbook
rinpol	249.00	NIST Webbook
rinpol	248.90	NIST Webbook
rinpol	248.75	NIST Webbook
rinpol	249.20	NIST Webbook
rinpol	240.45	NIST Webbook
rinpol	247.40	NIST Webbook

rinpol	253.15		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1422.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1418.54		NIST Webbook
rinpol	1424.62		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1425.03		NIST Webbook
rinpol	245.40		NIST Webbook
rinpol	1460.00		NIST Webbook
ripol	2193.00		NIST Webbook
ripol	2188.00		NIST Webbook
ripol	249.77		NIST Webbook
tb	553.20	K	NIST Webbook
tb	543.00 ± 5.00	K	NIST Webbook
tc	779.55	K	Joback Method
tf	366.40 ± 0.30	K	NIST Webbook
tf	362.60 ± 0.20	K	NIST Webbook
tf	365.50 ± 0.50	K	NIST Webbook
tf	364.90	K	Aqueous Solubility Prediction Method
tf	365.70 ± 2.00	K	NIST Webbook
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.61	J/mol×K	779.55	Joback Method
cpg	315.39	J/mol×K	738.94	Joback Method
cpg	306.52	J/mol×K	698.33	Joback Method
cpg	296.86	J/mol×K	657.72	Joback Method
cpg	286.28	J/mol×K	617.10	Joback Method
cpg	274.62	J/mol×K	576.49	Joback Method
cpg	261.76	J/mol×K	535.88	Joback Method
cps	166.40	J/mol×K	298.00	NIST Webbook
dvisc	0.0012738	Pa×s	335.62	Joback Method
dvisc	0.0007329	Pa×s	535.88	Joback Method
dvisc	0.0009068	Pa×s	435.75	Joback Method
dvisc	0.0008362	Pa×s	469.13	Joback Method
dvisc	0.0007794	Pa×s	502.50	Joback Method
dvisc	0.0011143	Pa×s	369.00	Joback Method

dvisc	0.0009967	Pa×s	402.37	Joback Method
hfust	6.94	kJ/mol	362.60	NIST Webbook
hfust	10.96	kJ/mol	362.00	NIST Webbook
hsubt	77.20	kJ/mol	383.00	NIST Webbook
hsubt	73.20 ± 0.50	kJ/mol	280.50	NIST Webbook
hsubt	71.10 ± 1.30	kJ/mol	302.00	NIST Webbook
psub	3.45e-03	kPa	314.80	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	3.47e-03	kPa	318.60	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	4.14e-03	kPa	319.70	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	3.45e-03	kPa	318.50	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	1.82e-03	kPa	311.90	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	1.14e-03	kPa	306.70	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method

psub	1.08e-03	kPa	304.70	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	5.31e-04	kPa	297.60	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	4.88e-04	kPa	297.40	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	1.05e-03	kPa	304.60	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
sfust	19.14	J/mol×K	362.60	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	431.00 ± 2.00	K	3.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.17908e+01

Coeff. B	-6.76309e+03
Coeff. C	-8.89840e+01
Temperature range (K), min.	403.50
Temperature range (K), max.	499.38

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C208968&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Recommended vapor pressures for acenaphthylene, fluoranthene, and fluorene.:	https://www.doi.org/10.1016/j.fluid.2016.11.012
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
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solubility of Acenaphthylene in Different Solvents between (278 and 329)K.:	https://www.doi.org/10.1021/je700347h
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume