Carbazole

Other names:	9-Azafluorene
	9H-Carbazole
	DIPHENYLENIMINE
	Dibenzo[b,d]pyrrole
	Dibenzopyrrole
	Diphenyleneimine
	Diphenylenimide
	NSC 3498
	SKF 20091
	USAF EK-600
Inchi:	InChI=1S/C12H9N/c1-3-7-11-9(5-1)10-6-2-4-8-12(10)13-11/h1-8,13H
InchiKey:	UJOBWOGCFQCDNV-UHFFFAOYSA-N
Formula:	C12H9N
SMILES:	c1ccc2c(c1)[nH]c1ccccc12
Mol. weight [g/mol]:	167.21
CAS:	86-74-8

Physical Properties

Property code	Value	Unit	Source
chs	-6133.50 ± 3.60	kJ/mol	NIST Webbook
chs	-6116.20	kJ/mol	NIST Webbook
chs	-6120.10 ± 3.40	kJ/mol	NIST Webbook
chs	-6110.10 ± 2.30	kJ/mol	NIST Webbook
hf	205.00 ± 3.00	kJ/mol	NIST Webbook
hf	222.90	kJ/mol	NIST Webbook
hf	209.60 ± 3.50	kJ/mol	NIST Webbook
hfs	125.10 ± 3.60	kJ/mol	NIST Webbook
hfs	111.80 ± 3.50	kJ/mol	NIST Webbook
hfs	101.70 ± 2.80	kJ/mol	NIST Webbook
hsub	103.30 ± 1.10	kJ/mol	NIST Webbook
hsub	103.30	kJ/mol	NIST Webbook
hsub	103.30 ± 1.10	kJ/mol	NIST Webbook
hsub	97.80	kJ/mol	NIST Webbook
hsub	97.70 ± 0.30	kJ/mol	NIST Webbook
hsub	97.70 ± 0.30	kJ/mol	NIST Webbook
hsub	109.00	kJ/mol	NIST Webbook
ie	7.68	eV	NIST Webbook

ie	7.57 ± 0.03	eV	NIST Webbook
ie	7.60 ± 0.10	eV	NIST Webbook
ie	7.20 ± 0.10	eV	NIST Webbook
ie	7.50	eV	NIST Webbook
log10ws	-5.27		Estimated Solubility Method
log10ws	-4.97		Aqueous Solubility Prediction Method
logp	2.839		Crippen Method
mcvol	131.540	ml/mol	McGowan Method
pc	3930.00	kPa	KDB
rinpol	1851.00		NIST Webbook
rinpol	1784.00		NIST Webbook
rinpol	1801.10		NIST Webbook
rinpol	1820.50		NIST Webbook
rinpol	1810.00		NIST Webbook
rinpol	1761.10		NIST Webbook
rinpol	1806.00		NIST Webbook
rinpol	1836.00		NIST Webbook
rinpol	1766.00		NIST Webbook
rinpol	1838.00		NIST Webbook
rinpol	1781.00		NIST Webbook
rinpol	1789.00		NIST Webbook
rinpol	1841.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1768.00		NIST Webbook
rinpol	1849.00		NIST Webbook
rinpol	1852.00		NIST Webbook
rinpol	1784.00		NIST Webbook
rinpol	308.63		NIST Webbook
rinpol	309.24		NIST Webbook
rinpol	310.15		NIST Webbook
rinpol	309.63		NIST Webbook
rinpol	310.35		NIST Webbook
rinpol	309.22		NIST Webbook
rinpol	311.71		NIST Webbook
rinpol	312.13		NIST Webbook
rinpol	309.80		NIST Webbook
rinpol	309.80		NIST Webbook
rinpol	310.35		NIST Webbook
rinpol	311.71		NIST Webbook
rinpol	307.90		NIST Webbook
rinpol	312.13		NIST Webbook
rinpol	309.02		NIST Webbook
rinpol	311.00		NIST Webbook

rinpol	314.30		NIST Webbook
rinpol	1801.10		NIST Webbook
rinpol	1836.00		NIST Webbook
rinpol	1823.00		NIST Webbook
rinpol	1823.00		NIST Webbook
rinpol	1784.00		NIST Webbook
tb	628.20	K	NIST Webbook
tb	627.85	K	KDB
tc	901.80	K	KDB
tf	517.04	K	Ternary phase diagram of phenanthrene and carbazole in different solvents and its application in the separation of them
tf	518.58	K	Aqueous Solubility Prediction Method
tf	519.30	K	KDB
vc	0.502	m3/kmol	KDB
zc	0.2631170		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	190.80	J/mol×K	298.15	NIST Webbook
cps	194.00	J/mol×K	298.15	NIST Webbook
hfust	27.20	kJ/mol	521.00	NIST Webbook
hfust	27.20	kJ/mol	516.00	NIST Webbook
hfust	26.90	kJ/mol	518.70	NIST Webbook
hfust	27.20	kJ/mol	521.10	NIST Webbook
hfust	27.08	kJ/mol	518.33	NIST Webbook
hsubt	101.20 ± 1.10	kJ/mol	355.00	NIST Webbook
hvapt	66.00	kJ/mol	570.50	NIST Webbook
hvapt	60.80	kJ/mol	605.00	NIST Webbook
hvapt	61.80	kJ/mol	565.00	NIST Webbook
hvapt	63.30	kJ/mol	525.00	NIST Webbook
hvapt	65.70	kJ/mol	578.00	NIST Webbook
sfust	52.19	J/mol×K	521.10	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	473.20	K	19.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51554e+01
Coeff. B	-5.84618e+03
Coeff. C	-7.33790e+01
Temperature range (K), min.	466.59
Temperature range (K), max.	667.27

Sources

Solid-liquid equilibrium of some polycyclic aromatic hydrocarbons in ethanol:	https://www.doi.org/10.1016/j.fluid.2012.01.031
Ternary phase diagram of phenanthrene and carbazole in different solvents and its application in the separation of them:	https://www.doi.org/10.1016/j.jct.2018.11.025
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C86748&Units=SI
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solid-liquid phase equilibrium of 9-fluorenone and several polynuclear aromatic hydrocarbons:	https://www.doi.org/10.1016/j.fluid.2012.01.017
Measurement and Modeling of the Solubility of 9H-Carbazole in Sub- and Supercritical Propane:	https://www.doi.org/10.1021/je100923d
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1373.mol
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Measurement and Modeling of the Solubility of Anthracene and Carbazole in Compressed Isobutane:	https://www.doi.org/10.1021/je300430d
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation 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
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
pvap:	Vapor pressure
rinpol:	Non-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
zc:	Critical Compressibility

Latest version available from:
https://www.chemeo.com/cid/63-782-4/Carbazole.pdf
Generated by Cheméo on 2024-04-20 06:55:39.679446495 +0000 UTC m=+15885388.600023810.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.