9H-Carbazole, 9-methyl-

Other names:	9-methyl-9H-carbazole
	9-methylcarbazole
	N-Methyldibenzopyrrole
	N-methylcarbazole
	NSC 121195
	carbazole, 9-methyl-
	carbazole, 9H-, 9-methyl-
Inchi:	InChI=1S/C13H11N/c1-14-12-8-4-2-6-10(12)11-7-3-5-9-13(11)14/h2-9H,1H3
InchiKey:	SDFLTYHTFPTIGX-UHFFFAOYSA-N
Formula:	C13H11N
SMILES:	Cn1c2ccccc2c2ccccc21
Mol. weight [g/mol]:	181.23
CAS:	1484-12-4

Physical Properties

Property code	Value	Unit	Source
chs	-6791.40 ± 1.70	kJ/mol	NIST Webbook
chs	-6793.18 ± 0.84	kJ/mol	NIST Webbook
hf	201.00	kJ/mol	NIST Webbook
hf	199.20 ± 2.40	kJ/mol	NIST Webbook
hf	199.10 ± 0.50	kJ/mol	NIST Webbook
hfs	105.50 ± 1.00	kJ/mol	NIST Webbook
hfs	103.70 ± 2.40	kJ/mol	NIST Webbook
hsub	95.50	kJ/mol	NIST Webbook
hsub	95.50	kJ/mol	NIST Webbook
hvap	79.50 ± 3.20	kJ/mol	NIST Webbook
ie	7.50 ± 0.10	eV	NIST Webbook
log10ws	-6.37		Crippen Method
logp	3.332		Crippen Method
mcvol	145.630	ml/mol	McGowan Method
rinpol	1738.80		NIST Webbook
rinpol	1750.20		NIST Webbook
ripol	2755.00		NIST Webbook
ripol	2805.00		NIST Webbook
ss	236.05	J/mol×K	NIST Webbook
ss	234.30	J/mol×K	NIST Webbook
ss	234.30	J/mol×K	NIST Webbook

ss	234.30	J/mol×K	NIST Webbook
tt	362.49 ± 0.03	K	NIST Webbook
tt	362.48 ± 0.04	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	217.84	J/mol×K	298.15	NIST Webbook
cps	217.84	J/mol×K	298.15	NIST Webbook
cps	204.80	J/mol×K	298.15	NIST Webbook
cps	218.42	J/mol×K	298.15	NIST Webbook
cps	217.84	J/mol×K	298.15	NIST Webbook
hfust	17.15	kJ/mol	362.49	NIST Webbook
hfust	17.15	kJ/mol	362.50	NIST Webbook
hfust	17.15	kJ/mol	362.50	NIST Webbook
hfust	17.15	kJ/mol	362.49	NIST Webbook
hsubt	95.00	kJ/mol	322.50	NIST Webbook
hsubt	95.50 ± 0.30	kJ/mol	95.50	NIST Webbook
hvapt	74.90	kJ/mol	366.00	NIST Webbook
hvapt	70.50	kJ/mol	523.00	NIST Webbook
hvapt	55.90	kJ/mol	523.00	NIST Webbook
hvapt	59.10	kJ/mol	523.00	NIST Webbook
hvapt	62.10	kJ/mol	523.00	NIST Webbook
hvapt	65.00	kJ/mol	523.00	NIST Webbook
hvapt	67.70	kJ/mol	523.00	NIST Webbook
hvapt	73.40	kJ/mol	523.00	NIST Webbook
hvapt	79.40	kJ/mol	298.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Heterocycles and Related Compounds
sfust	47.32	J/mol×K	362.49	NIST Webbook
sfust	47.32	J/mol×K	362.49	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1484124&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Heterocycles and Related Compounds:	https://www.doi.org/10.1021/je900034d
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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
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
tt:	Triple Point Temperature

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