

1-METHYLCARBAZOLE

Other names:	9H-Carbazole, 1-methyl- Carbazole, 1-methyl
Inchi:	InChI=1S/C13H11N/c1-9-5-4-7-11-10-6-2-3-8-12(10)14-13(9)11/h2-8,14H,1H3
InchiKey:	HIAGSPVAYSSKHL-UHFFFAOYSA-N
Formula:	C13H11N
SMILES:	Cc1cccc2c1[nH]c1cccc12
Mol. weight [g/mol]:	181.24

Physical Properties

Property code	Value	Unit	Source
af	0.4949		Cheméo Relay (1.0)
gf	301.34	kJ/mol	Cheméo Relay (1.0, beta)
hf	182.85	kJ/mol	Cheméo Relay (1.0)
hvap	88.58	kJ/mol	Cheméo Relay (1.0)
ie	7.23	eV	Cheméo Relay (1.0)
log10ws	-4.64		Cheméo Relay (1.0)
logp	3.148		Crippen Method
mcvol	145.630	ml/mol	McGowan Method
pc	3770.50	kPa	Cheméo Relay (1.0, beta)
rinpol	324.45		NIST Webbook
tb	630.31	K	Cheméo Relay (1.0)
tc	915.34	K	Cheméo Relay (1.0)
tf	459.20	K	Cheméo Relay (1.0)
vc	0.552	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6510652&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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