

# N-Methyl-2,3-5,6-dibenzazalene

**Inchi:** InChI=1S/C17H13N/c1-18-16-9-5-3-7-13(16)10-15-14-8-4-2-6-12(14)11-17(15)18/h2-11H  
**InchiKey:** VMSTUPSUMJBRGU-UHFFFAOYSA-N  
**Formula:** C17H13N  
**SMILES:** Cn1c2cc3ccccc3c-2cc2ccccc21  
**Mol. weight [g/mol]:** 231.29  
**CAS:** 6626-64-8

## Physical Properties

Property code	Value	Unit	Source
chs	-8752.90	kJ/mol	NIST Webbook
hf	337.00	kJ/mol	NIST Webbook
hsub	132.00	kJ/mol	NIST Webbook
log10ws	-8.39		Crippen Method
logp	4.436		Crippen Method
mcvol	182.530	ml/mol	McGowan Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	122.20	kJ/mol	381.50	NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C6626648&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

# Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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