

# 9,10-Anthracenedicarbonitrile

<b>Other names:</b>	9,10-Dicyanoanthracene 9,10-Dicyanoanthracen
<b>Inchi:</b>	InChI=1S/C16H8N2/c17-9-15-11-5-1-2-6-12(11)16(10-18)14-8-4-3-7-13(14)15/h1-8H
<b>InchiKey:</b>	BIOPPFDHKHWJIA-UHFFFAOYSA-N
<b>Formula:</b>	C16H8N2
<b>SMILES:</b>	N#Cc1c2cccc2c(C#N)c2cccc12
<b>Mol. weight [g/mol]:</b>	228.25
<b>CAS:</b>	1217-45-4

## Physical Properties

Property code	Value	Unit	Source
gf	647.02	kJ/mol	Joback Method
hf	540.45	kJ/mol	Joback Method
hfus	27.12	kJ/mol	Joback Method
hvap	79.71	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	3.736		Crippen Method
mcvol	176.380	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinqol	2288.00		NIST Webbook
rinqol	2288.00		NIST Webbook
rinqol	2288.00		NIST Webbook
tb	849.22	K	Joback Method
tc	1112.96	K	Joback Method
tf	529.44	K	Joback Method
vc	0.720	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.63	J/molxK	849.22	Joback Method
cpg	467.21	J/molxK	893.18	Joback Method
cpg	476.25	J/molxK	937.13	Joback Method
cpg	484.90	J/molxK	981.09	Joback Method

cpg	493.29	J/mol×K	1025.05	Joback Method
cpg	501.58	J/mol×K	1069.00	Joback Method
cpg	509.90	J/mol×K	1112.96	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1217454&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1217454&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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