

# 2-Nitroanthracene

<b>Inchi:</b>	InChI=1S/C14H9NO2/c16-15(17)14-6-5-12-7-10-3-1-2-4-11(10)8-13(12)9-14/h1-9H
<b>InchiKey:</b>	NZWGQBVOKEKLD-UHFFFAOYSA-N
<b>Formula:</b>	C14H9NO2
<b>SMILES:</b>	O=[N+]([O-])c1ccc2cc3ccccc3cc2c1
<b>Mol. weight [g/mol]:</b>	223.23
<b>CAS:</b>	3586-69-4

## Physical Properties

Property code	Value	Unit	Source
gf	409.00	kJ/mol	Joback Method
hf	252.68	kJ/mol	Joback Method
hfus	30.68	kJ/mol	Joback Method
hvap	70.23	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	3.901		Crippen Method
mcvol	162.860	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
rinpol	379.65		NIST Webbook
rinpol	379.65		NIST Webbook
rinpol	379.46		NIST Webbook
tb	746.16	K	Joback Method
tc	1021.21	K	Joback Method
tf	508.01	K	Joback Method
vc	0.637	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.33	J/molxK	746.16	Joback Method
cpg	436.51	J/molxK	792.00	Joback Method
cpg	447.68	J/molxK	837.84	Joback Method
cpg	458.00	J/molxK	883.68	Joback Method
cpg	467.67	J/molxK	929.53	Joback Method
cpg	476.86	J/molxK	975.37	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3586694&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3586694&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>

## 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>mccvol:</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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