

# 1-Aminophenanthrene

<b>Inchi:</b>	InChI=1S/C14H11N/c15-14-7-3-6-12-11-5-2-1-4-10(11)8-9-13(12)14/h1-9H,15H2
<b>InchiKey:</b>	CXZOCEZMGWOOFD-UHFFFAOYSA-N
<b>Formula:</b>	C14H11N
<b>SMILES:</b>	Nc1cccc2c1ccc1ccccc12
<b>Mol. weight [g/mol]:</b>	193.24
<b>CAS:</b>	4176-53-8

## Physical Properties

Property code	Value	Unit	Source
gf	439.90	kJ/mol	Joback Method
hf	297.23	kJ/mol	Joback Method
hfus	24.51	kJ/mol	Joback Method
hvap	64.28	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	3.575		Crippen Method
mcvol	155.420	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
rinpol	362.62		NIST Webbook
rinpol	356.21		NIST Webbook
rinpol	356.21		NIST Webbook
tb	666.85	K	Joback Method
tc	927.60	K	Joback Method
tf	447.66	K	Joback Method
vc	0.585	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.28	J/molxK	666.85	Joback Method
cpg	402.87	J/molxK	710.31	Joback Method
cpg	415.31	J/molxK	753.77	Joback Method
cpg	426.75	J/molxK	797.22	Joback Method
cpg	437.35	J/molxK	840.68	Joback Method
cpg	447.26	J/molxK	884.14	Joback Method

## Sources

<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=C4176538&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4176538&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>

## 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>mcvol:</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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