

# 1-Amino-8-nitropyrene

<b>Inchi:</b>	InChI=1S/C16H10N2O2/c17-13-7-3-9-1-2-10-4-8-14(18(19)20)12-6-5-11(13)15(9)16(10)
<b>InchiKey:</b>	WGVCNGPAJHVJJK-UHFFFAOYSA-N
<b>Formula:</b>	C16H10N2O2
<b>SMILES:</b>	<chem>Nc1ccc2ccc3ccc([N+](=O)[O-])c4ccc1c2c34</chem>
<b>Mol. weight [g/mol]:</b>	262.26
<b>CAS:</b>	30269-02-4

## Physical Properties

Property code	Value	Unit	Source
gf	573.92	kJ/mol	Joback Method
hf	367.86	kJ/mol	Joback Method
hfus	40.27	kJ/mol	Joback Method
hvap	87.65	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	4.074		Crippen Method
mcvol	185.860	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
rinpol	3217.00		NIST Webbook
rinpol	3217.00		NIST Webbook
tb	885.69	K	Joback Method
tc	1162.60	K	Joback Method
tf	677.83	K	Joback Method
vc	0.731	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.08	J/molxK	885.69	Joback Method
cpg	535.30	J/molxK	931.84	Joback Method
cpg	546.38	J/molxK	977.99	Joback Method
cpg	557.58	J/molxK	1024.15	Joback Method
cpg	569.17	J/molxK	1070.30	Joback Method
cpg	581.38	J/molxK	1116.45	Joback Method
cpg	594.49	J/molxK	1162.60	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=C30269024&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C30269024&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>hvp:</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>rinp:</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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