

# 9-Methyl-10-nitroanthracene

<b>Inchi:</b>	InChI=1S/C15H11NO2/c1-10-11-6-2-4-8-13(11)15(16(17)18)14-9-5-3-7-12(10)14/h2-9H,
<b>InchiKey:</b>	FMIFGOKEBFQCGG-UHFFFAOYSA-N
<b>Formula:</b>	C15H11NO2
<b>SMILES:</b>	<chem>Cc1c2ccccc2c([N+](=O)[O-])c2ccccc12</chem>
<b>Mol. weight [g/mol]:</b>	237.25
<b>CAS:</b>	84457-22-7

## Physical Properties

Property code	Value	Unit	Source
gf	407.79	kJ/mol	Joback Method
hf	220.57	kJ/mol	Joback Method
hfus	32.88	kJ/mol	Joback Method
hvap	73.12	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	4.210		Crippen Method
mvol	176.950	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	383.31		NIST Webbook
rinpol	382.88		NIST Webbook
tb	774.02	K	Joback Method
tc	1042.99	K	Joback Method
tf	531.80	K	Joback Method
vc	0.694	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.29	J/molxK	774.02	Joback Method
cpg	486.98	J/molxK	818.85	Joback Method
cpg	498.71	J/molxK	863.68	Joback Method
cpg	509.65	J/molxK	908.51	Joback Method
cpg	519.97	J/molxK	953.34	Joback Method
cpg	529.81	J/molxK	998.17	Joback Method
cpg	539.36	J/molxK	1042.99	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=C84457227&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C84457227&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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</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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