

# Phenanthrene, 3,9-dimethyl-

<b>Other names:</b>	3,9-dimethylphenanthrene
<b>Inchi:</b>	InChI=1S/C16H14/c1-11-7-8-13-10-12(2)14-5-3-4-6-15(14)16(13)9-11/h3-10H,1-2H3
<b>InchiKey:</b>	MXXOWAVGWFAQJHQ-UHFFFAOYSA-N
<b>Formula:</b>	C16H14
<b>SMILES:</b>	<chem>Cc1ccc2cc(C)c3ccccc3c2c1</chem>
<b>Mol. weight [g/mol]:</b>	206.28
<b>CAS:</b>	66291-32-5

## Physical Properties

Property code	Value	Unit	Source
gf	380.66	kJ/mol	Joback Method
hf	210.69	kJ/mol	Joback Method
hfus	24.11	kJ/mol	Joback Method
hvap	58.75	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	4.610		Crippen Method
mcvol	173.620	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	339.65		NIST Webbook
rinpol	341.50		NIST Webbook
rinpol	340.20		NIST Webbook
rinpol	341.40		NIST Webbook
rinpol	341.75		NIST Webbook
rinpol	340.79		NIST Webbook
rinpol	2011.00		NIST Webbook
rinpol	340.60		NIST Webbook
tb	645.06	K	Joback Method
tc	889.67	K	Joback Method
tf	399.46	K	Joback Method
vc	0.667	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	429.69	J/molxK	645.06	Joback Method
cpg	497.31	J/molxK	848.90	Joback Method
cpg	485.63	J/molxK	808.13	Joback Method
cpg	473.15	J/molxK	767.36	Joback Method
cpg	459.74	J/molxK	726.60	Joback Method
cpg	445.30	J/molxK	685.83	Joback Method
cpg	508.31	J/molxK	889.67	Joback Method
dvisc	0.0004320	Paxs	645.06	Joback Method
dvisc	0.0004850	Paxs	604.13	Joback Method
dvisc	0.0005537	Paxs	563.19	Joback Method
dvisc	0.0006454	Paxs	522.26	Joback Method
dvisc	0.0007722	Paxs	481.33	Joback Method
dvisc	0.0009553	Paxs	440.39	Joback Method
dvisc	0.0012344	Paxs	399.46	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=C66291325&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C66291325&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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

**tf:** Normal melting (fusion) point

**vc:** Critical Volume

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