

# Phenanthrene, 9-ethyl-

<b>Other names:</b>	9-Ethylphenanthrene
<b>Inchi:</b>	InChI=1S/C16H14/c1-2-12-11-13-7-3-4-9-15(13)16-10-6-5-8-14(12)16/h3-11H,2H2,1H3
<b>InchiKey:</b>	ZWANHXINCHPSIK-UHFFFAOYSA-N
<b>Formula:</b>	C16H14
<b>SMILES:</b>	CCc1cc2ccccc2c2ccccc12
<b>Mol. weight [g/mol]:</b>	206.28
<b>CAS:</b>	3674-75-7

## Physical Properties

Property code	Value	Unit	Source
gf	390.29	kJ/mol	Joback Method
hf	222.16	kJ/mol	Joback Method
hfus	24.50	kJ/mol	Joback Method
hvap	58.09	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.555		Crippen Method
mcvol	173.620	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
rinpol	337.00		NIST Webbook
rinpol	335.40		NIST Webbook
rinpol	337.05		NIST Webbook
rinpol	335.46		NIST Webbook
rinpol	336.46		NIST Webbook
rinpol	336.98		NIST Webbook
rinpol	336.41		NIST Webbook
rinpol	337.05		NIST Webbook
rinpol	335.46		NIST Webbook
rinpol	337.05		NIST Webbook
rinpol	335.40		NIST Webbook
rinpol	337.05		NIST Webbook
rinpol	336.60		NIST Webbook
tb	640.08	K	Joback Method
tc	883.76	K	Joback Method
tf	386.94	K	Joback Method
vc	0.667	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.53	J/molxK	640.08	Joback Method
cpg	446.38	J/molxK	680.69	Joback Method
cpg	461.00	J/molxK	721.31	Joback Method
cpg	474.53	J/molxK	761.92	Joback Method
cpg	487.10	J/molxK	802.53	Joback Method
cpg	498.83	J/molxK	843.15	Joback Method
cpg	509.85	J/molxK	883.76	Joback Method
dvisc	0.0014025	Paxs	386.94	Joback Method
dvisc	0.0010464	Paxs	429.13	Joback Method
dvisc	0.0008227	Paxs	471.32	Joback Method
dvisc	0.0006730	Paxs	513.51	Joback Method
dvisc	0.0005675	Paxs	555.70	Joback Method
dvisc	0.0004902	Paxs	597.89	Joback Method
dvisc	0.0004317	Paxs	640.08	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.37543e+01
Coeff. B	-4.78678e+03
Coeff. C	-1.19348e+02
Temperature range (K), min.	474.80
Temperature range (K), max.	686.31

## Sources

<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=C3674757&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3674757&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
<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>

## 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>pvap:</b>	Vapor 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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