

# Naphtho[2,3-g]chrysene

<b>Inchi:</b>	InChI=1S/C26H16/c1-2-9-19-16-25-24(15-18(19)8-1)22-12-6-5-11-21(22)23-14-13-17-7-3
<b>InchiKey:</b>	JBHIIKGZANVCJJ-UHFFFAOYSA-N
<b>Formula:</b>	C26H16
<b>SMILES:</b>	<chem>c1ccc2cc3c(cc2c1)c1cccc1c1ccc2ccccc2c13</chem>
<b>Mol. weight [g/mol]:</b>	328.41
<b>CAS:</b>	196-64-5

## Physical Properties

Property code	Value	Unit	Source
gf	775.18	kJ/mol	Joback Method
hf	566.03	kJ/mol	Joback Method
hfus	40.68	kJ/mol	Joback Method
hvap	86.59	kJ/mol	Joback Method
ie	7.15 ± 0.04	eV	NIST Webbook
ie	7.15 ± 0.02	eV	NIST Webbook
log10ws	-10.49		Crippen Method
logp	7.453		Crippen Method
mcvol	256.140	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpola	575.96		NIST Webbook
rinpola	567.36		NIST Webbook
tb	935.78	K	Joback Method
tc	1209.93	K	Joback Method
tf	622.78	K	Joback Method
vc	0.994	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.48	J/mol×K	935.78	Joback Method
cpg	769.57	J/mol×K	981.47	Joback Method
cpg	785.72	J/mol×K	1027.16	Joback Method
cpg	802.30	J/mol×K	1072.85	Joback Method
cpg	819.68	J/mol×K	1118.55	Joback Method

cpg	838.20	J/mol×K	1164.24	Joback Method
cpg	858.23	J/mol×K	1209.93	Joback Method
dvisc	0.0031676	Paxs	622.78	Joback Method
dvisc	0.0027637	Paxs	674.95	Joback Method
dvisc	0.0024589	Paxs	727.11	Joback Method
dvisc	0.0022223	Paxs	779.28	Joback Method
dvisc	0.0020341	Paxs	831.45	Joback Method
dvisc	0.0018814	Paxs	883.61	Joback Method
dvisc	0.0017553	Paxs	935.78	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=C196645&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C196645&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>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</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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