

# Dibenzo[a,n]picene

<b>Inchi:</b>	InChI=1S/C30H18/c1-2-7-22-18-29-23(17-21(22)6-1)12-14-25-26-13-11-20-10-9-19-5-3-
<b>InchiKey:</b>	SMHZBBHLTQNHOT-UHFFFAOYSA-N
<b>Formula:</b>	C30H18
<b>SMILES:</b>	<chem>c1ccc2cc3c(ccc4c3ccc3c4ccc4ccc5ccccc5c43)cc2c1</chem>
<b>Mol. weight [g/mol]:</b>	378.46
<b>CAS:</b>	115747-62-1

## Physical Properties

Property code	Value	Unit	Source
gf	905.88	kJ/mol	Joback Method
hf	663.07	kJ/mol	Joback Method
hfus	47.67	kJ/mol	Joback Method
hvap	97.80	kJ/mol	Joback Method
log10ws	-12.30		Crippen Method
logp	8.606		Crippen Method
mcvol	293.040	ml/mol	McGowan Method
pc	1777.34	kPa	Joback Method
tb	1051.26	K	Joback Method
tc	1330.47	K	Joback Method
tf	713.08	K	Joback Method
vc	1.139	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.76	J/molxK	1051.26	Joback Method
cpg	929.78	J/molxK	1097.80	Joback Method
cpg	951.06	J/molxK	1144.33	Joback Method
cpg	974.05	J/molxK	1190.87	Joback Method
cpg	999.18	J/molxK	1237.40	Joback Method
cpg	1026.90	J/molxK	1283.94	Joback Method
cpg	1057.66	J/molxK	1330.47	Joback Method
dvisc	0.0046199	Paxs	713.08	Joback Method
dvisc	0.0041148	Paxs	769.44	Joback Method

dvisc	0.0037234	Paxs	825.81	Joback Method
dvisc	0.0034125	Paxs	882.17	Joback Method
dvisc	0.0031604	Paxs	938.53	Joback Method
dvisc	0.0029526	Paxs	994.90	Joback Method
dvisc	0.0027786	Paxs	1051.26	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=C115747621&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C115747621&amp;Units=SI</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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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