

# Benz[a]anthracene, 7,12-dimethyl-

**Other names:**

1,4-Dimethyl-2,3-benzphenanthrene  
6,7-Dimethyl-1,2-benzanthracene  
7,12-DMBA  
7,12-Dimethyl-1,2-benzanthracene  
7,12-Dimethylbenz(a)anthracene  
7,12-Dimethylbenz[a]anthracene  
7,12-Dimethylbenzanthracene  
7,12-Dimethylbenzo[a]anthracene  
7,12-dimethylbenzo[b]phenanthrene  
9,10-Dimethyl-1,2-benzanthracene  
9,10-Dimethyl-1,2-benzanthrazen  
9,10-Dimethylbenz[a]anthracene  
Benz(a)anthracene, 9,10-dimethyl-  
DMBA  
NCI-C03918  
NSC 408823

**Inchi:**

InChI=1S/C20H16/c1-13-16-8-5-6-9-17(16)14(2)20-18(13)12-11-15-7-3-4-10-19(15)20/h

**InchiKey:**

ARSRBNBHOADGJU-UHFFFAOYSA-N

**Formula:**

C20H16

**SMILES:**

Cc1c2ccccc2c(C)c2c1ccc1cccc12

**Mol. weight [g/mol]:**

256.34

**CAS:**

57-97-6

## Physical Properties

Property code	Value	Unit	Source
gf	511.36	kJ/mol	Joback Method
hf	307.73	kJ/mol	Joback Method
hfus	31.10	kJ/mol	Joback Method
hvap	69.96	kJ/mol	Joback Method
ie	7.43	eV	NIST Webbook
ie	7.10 ± 0.03	eV	NIST Webbook
log10ws	-7.02		Aqueous Solubility Prediction Method
log10ws	-7.02		Estimated Solubility Method
logp	5.763		Crippen Method
mvol	210.520	ml/mol	McGowan Method

pc	2200.01	kPa	Joback Method
rinpol	2711.00		NIST Webbook
rinpol	444.84		NIST Webbook
rinpol	443.38		NIST Webbook
rinpol	442.03		NIST Webbook
rinpol	2711.00		NIST Webbook
rinpol	2713.00		NIST Webbook
rinpol	443.90		NIST Webbook
rinpol	443.82		NIST Webbook
rinpol	444.00		NIST Webbook
rinpol	443.38		NIST Webbook
tb	760.54	K	Joback Method
tc	1013.66	K	Joback Method
tf	395.65	K	Aqueous Solubility Prediction Method
vc	0.814	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.63	J/molxK	760.54	Joback Method
cpg	586.13	J/molxK	802.73	Joback Method
cpg	600.62	J/molxK	844.91	Joback Method
cpg	614.28	J/molxK	887.10	Joback Method
cpg	627.28	J/molxK	929.28	Joback Method
cpg	639.81	J/molxK	971.47	Joback Method
cpg	652.05	J/molxK	1013.66	Joback Method
dvisc	0.0014862	Paxs	489.76	Joback Method
dvisc	0.0012234	Paxs	534.89	Joback Method
dvisc	0.0010381	Paxs	580.02	Joback Method
dvisc	0.0009019	Paxs	625.15	Joback Method
dvisc	0.0007987	Paxs	670.28	Joback Method
dvisc	0.0007181	Paxs	715.41	Joback Method
dvisc	0.0006539	Paxs	760.54	Joback Method

## Correlations

Information

Value

Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.52074e+01
Coeff. B	-7.83311e+03
Temperature range (K), min.	525.01
Temperature range (K), max.	791.55

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C57976&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C57976&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</a>
<b>Estimated Solubility Method:</b>	<a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor 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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