

# 1-Methylbenzo(a)pyrene

<b>Inchi:</b>	InChI=1S/C21H14/c1-13-6-7-14-8-9-16-12-15-4-2-3-5-18(15)19-11-10-17(13)20(14)21(1)
<b>InchiKey:</b>	WMAYPBMLSQKCHA-UHFFFAOYSA-N
<b>Formula:</b>	C21H14
<b>SMILES:</b>	Cc1ccc2ccc3cc4ccccc4c4ccc1c2c34
<b>Mol. weight [g/mol]:</b>	266.34
<b>CAS:</b>	40568-90-9

## Physical Properties

Property code	Value	Unit	Source
gf	620.67	kJ/mol	Joback Method
hf	432.70	kJ/mol	Joback Method
hfus	33.68	kJ/mol	Joback Method
hvap	73.19	kJ/mol	Joback Method
log10ws	-8.58		Crippen Method
logp	6.046		Crippen Method
mvol	209.450	ml/mol	McGowan Method
pc	2336.03	kPa	Joback Method
rinpol	473.70		NIST Webbook
tb	794.70	K	Joback Method
tc	1053.20	K	Joback Method
tf	540.01	K	Joback Method
vc	0.822	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.91	J/molxK	794.70	Joback Method
cpg	586.99	J/molxK	837.78	Joback Method
cpg	600.46	J/molxK	880.87	Joback Method
cpg	613.57	J/molxK	923.95	Joback Method
cpg	626.59	J/molxK	967.03	Joback Method
cpg	639.79	J/molxK	1010.12	Joback Method
cpg	653.41	J/molxK	1053.20	Joback Method
dvisc	0.0031877	Paxs	540.01	Joback Method

dvisc	0.0029417	Paxs	582.46	Joback Method
dvisc	0.0027446	Paxs	624.91	Joback Method
dvisc	0.0025833	Paxs	667.36	Joback Method
dvisc	0.0024492	Paxs	709.80	Joback Method
dvisc	0.0023360	Paxs	752.25	Joback Method
dvisc	0.0022394	Paxs	794.70	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C40568909&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C40568909&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>
<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>

## 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
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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