

# 1,4:5,8:9,10-Trimethanoanthracene, 1,2,3,4,4a,5,8,8a,9,9a,10,10a-dodecahydro-(1 «alpha

Inchi:	InChI=1S/C17H22/c1-2-9-5-8(1)14-12-7-13(15(9)14)17-11-4-3-10(6-11)16(12)17/h1-2,8-
InchiKey:	FUCGLOJSPSEIKX-JDEKWYGUSA-N
Formula:	C17H22
SMILES:	C1=CC2CC1C1C3CC(C21)C1C2CCC(C2)C31
Mol. weight [g/mol]:	226.36
CAS:	87424-91-7

## Physical Properties

Property code	Value	Unit	Source
gf	467.98	kJ/mol	Joback Method
hf	25.17	kJ/mol	Joback Method
hfus	36.20	kJ/mol	Joback Method
hvap	51.80	kJ/mol	Joback Method
ie	8.68	eV	NIST Webbook
log10ws	-3.74		Crippen Method
logp	3.737		Crippen Method
mcvol	180.930	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
tb	605.01	K	Joback Method
tc	828.43	K	Joback Method
tf	376.31	K	Joback Method
vc	0.720	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.82	J/molxK	605.01	Joback Method
cpg	594.43	J/molxK	642.25	Joback Method
cpg	617.19	J/molxK	679.48	Joback Method
cpg	638.31	J/molxK	716.72	Joback Method
cpg	658.01	J/molxK	753.95	Joback Method
cpg	676.51	J/molxK	791.19	Joback Method
cpg	694.04	J/molxK	828.43	Joback Method
dvisc	0.0051736	Paxs	376.31	Joback Method

dvisc	0.0094937	Paxs	414.43	Joback Method
dvisc	0.0157277	Paxs	452.54	Joback Method
dvisc	0.0240900	Paxs	490.66	Joback Method
dvisc	0.0346984	Paxs	528.78	Joback Method
dvisc	0.0475853	Paxs	566.89	Joback Method
dvisc	0.0627123	Paxs	605.01	Joback Method

## 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=C87424917&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C87424917&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>mvol:</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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