

# 4,5,6-trihydrobenz[de]anthracene

<b>Inchi:</b>	InChI=1S/C17H14/c1-2-9-15-13(5-1)11-14-8-3-6-12-7-4-10-16(15)17(12)14/h1-3,5-6,8-9,
<b>InchiKey:</b>	QUOCOXLVRYLTP-UHFFFAOYSA-N
<b>Formula:</b>	C17H14
<b>SMILES:</b>	<chem>c1ccc2c3c4c(cccc4cc2c1)CCC3</chem>
<b>Mol. weight [g/mol]:</b>	218.29

## Physical Properties

Property code	Value	Unit	Source
gf	457.54	kJ/mol	Joback Method
hf	283.19	kJ/mol	Joback Method
hfus	23.76	kJ/mol	Joback Method
hvap	61.20	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	4.482		Crippen Method
mcvol	176.850	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
tb	679.35	K	Joback Method
tc	935.56	K	Joback Method
tf	432.91	K	Joback Method
vc	0.681	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.24	J/mol×K	679.35	Joback Method
cpg	478.18	J/mol×K	722.05	Joback Method
cpg	492.87	J/mol×K	764.75	Joback Method
cpg	506.49	J/mol×K	807.45	Joback Method
cpg	519.26	J/mol×K	850.15	Joback Method
cpg	531.38	J/mol×K	892.86	Joback Method
cpg	543.05	J/mol×K	935.56	Joback Method
dvisc	0.0020061	Paxs	432.91	Joback Method
dvisc	0.0016661	Paxs	473.98	Joback Method
dvisc	0.0014254	Paxs	515.06	Joback Method

dvisc	0.0012479	Paxs	556.13	Joback Method
dvisc	0.0011126	Paxs	597.20	Joback Method
dvisc	0.0010068	Paxs	638.28	Joback Method
dvisc	0.0009221	Paxs	679.35	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=R15511&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R15511&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>hvac:</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>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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