

# 3H-Benz[e]indene

<b>Inchi:</b>	InChI=1S/C13H10/c1-2-6-12-10(4-1)8-9-11-5-3-7-13(11)12/h1-4,6-9H,5H2
<b>InchiKey:</b>	USPJQUFZLZTSBK-UHFFFAOYSA-N
<b>Formula:</b>	C13H10
<b>SMILES:</b>	C1=Cc2c(ccc3ccccc23)C1
<b>Mol. weight [g/mol]:</b>	166.22
<b>CAS:</b>	232-55-3

## Physical Properties

Property code	Value	Unit	Source
gf	356.80	kJ/mol	Joback Method
hf	243.93	kJ/mol	Joback Method
hfus	17.99	kJ/mol	Joback Method
hvap	50.29	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.409		Crippen Method
mcvol	135.650	ml/mol	McGowan Method
pc	3376.28	kPa	Joback Method
tb	563.03	K	Joback Method
tc	810.68	K	Joback Method
tf	343.37	K	Joback Method
vc	0.521	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.80	J/mol×K	563.03	Joback Method
cpg	321.41	J/mol×K	604.30	Joback Method
cpg	334.73	J/mol×K	645.58	Joback Method
cpg	346.90	J/mol×K	686.85	Joback Method
cpg	358.06	J/mol×K	728.13	Joback Method
cpg	368.35	J/mol×K	769.40	Joback Method
cpg	377.92	J/mol×K	810.68	Joback Method
dvisc	0.0014835	Paxs	343.37	Joback Method
dvisc	0.0011839	Paxs	379.98	Joback Method

dvisc	0.0009831	Paxs	416.59	Joback Method
dvisc	0.0008412	Paxs	453.20	Joback Method
dvisc	0.0007367	Paxs	489.81	Joback Method
dvisc	0.0006572	Paxs	526.42	Joback Method
dvisc	0.0005951	Paxs	563.03	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=C232553&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C232553&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>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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