

# 5H-Dibenzo[a,d]cycloheptene

<b>Other names:</b>	Dibenzo[a,d]cycloheptatriene Dibenzo[a,e]cycloheptatriene Suberene 1,2:5,6-Dibenzcycloheptatriene 1,2:5,6-Dibenzotropilidene 2,3:6,7-Dibenzocycloheptatriene 2,3:6,7-Dibenzo-4-suberene Dibenzo[a,d]cycloheptene 5H-Dibenzo[a,d]cycloheptatriene
<b>Inchi:</b>	InChI=1S/C15H12/c1-3-7-14-11-15-8-4-2-6-13(15)10-9-12(14)5-1/h1-10H,11H2
<b>InchiKey:</b>	QPJORFLSOJAUNL-UHFFFAOYSA-N
<b>Formula:</b>	C15H12
<b>SMILES:</b>	<chem>C1=Cc2ccccc2Cc2ccccc21</chem>
<b>Mol. weight [g/mol]:</b>	192.26
<b>CAS:</b>	256-81-5

## Physical Properties

Property code	Value	Unit	Source
gf	379.40	kJ/mol	Joback Method
hf	248.11	kJ/mol	Joback Method
hfus	20.20	kJ/mol	Joback Method
hvap	55.37	kJ/mol	Joback Method
ie	7.60	eV	NIST Webbook
ie	7.95	eV	NIST Webbook
log10ws	-4.42		Crippen Method
logp	3.761		Crippen Method
mcvol	159.530	ml/mol	McGowan Method
pc	2995.87	kPa	Joback Method
tb	616.49	K	Joback Method
tc	873.57	K	Joback Method
tf	359.63	K	Joback Method
vc	0.604	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.27	J/molxK	616.49	Joback Method
cpg	399.78	J/molxK	659.34	Joback Method
cpg	414.86	J/molxK	702.18	Joback Method
cpg	428.65	J/molxK	745.03	Joback Method
cpg	441.30	J/molxK	787.87	Joback Method
cpg	452.94	J/molxK	830.72	Joback Method
cpg	463.71	J/molxK	873.57	Joback Method
dvisc	0.0016065	Paxs	359.63	Joback Method
dvisc	0.0010862	Paxs	402.44	Joback Method
dvisc	0.0007918	Paxs	445.25	Joback Method
dvisc	0.0006101	Paxs	488.06	Joback Method
dvisc	0.0004903	Paxs	530.87	Joback Method
dvisc	0.0004071	Paxs	573.68	Joback Method
dvisc	0.0003468	Paxs	616.49	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C256815&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C256815&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>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>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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