

# 1,3-Cyclopentadiene, 2-hexyl

Inchi:	InChI=1S/C11H18/c1-2-3-4-5-8-11-9-6-7-10-11/h6,9-10H,2-5,7-8H2,1H3
InchiKey:	POPBPNUXNUXOIX-UHFFFAOYSA-N
Formula:	C11H18
SMILES:	CCCCCCC1=CCC=C1
Mol. weight [g/mol]:	150.26

## Physical Properties

Property code	Value	Unit	Source
gf	136.29	kJ/mol	Joback Method
hf	-85.46	kJ/mol	Joback Method
hfus	19.17	kJ/mol	Joback Method
hvap	41.89	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.843		Crippen Method
mcvol	146.390	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
rinpola	1107.00		NIST Webbook
ripola	1302.00		NIST Webbook
tb	474.33	K	Joback Method
tc	666.96	K	Joback Method
tf	242.91	K	Joback Method
vc	0.566	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.14	J/molxK	474.33	Joback Method
cpg	332.41	J/molxK	506.44	Joback Method
cpg	347.84	J/molxK	538.54	Joback Method
cpg	362.47	J/molxK	570.65	Joback Method
cpg	376.34	J/molxK	602.75	Joback Method
cpg	389.47	J/molxK	634.86	Joback Method
cpg	401.90	J/molxK	666.96	Joback Method
dvisc	0.0033452	Paxs	242.91	Joback Method

dvisc	0.0016415	Paxs	281.48	Joback Method
dvisc	0.0009563	Paxs	320.05	Joback Method
dvisc	0.0006258	Paxs	358.62	Joback Method
dvisc	0.0004446	Paxs	397.19	Joback Method
dvisc	0.0003356	Paxs	435.76	Joback Method
dvisc	0.0002652	Paxs	474.33	Joback Method

## Sources

<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=R40845&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R40845&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>

## 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>ripol:</b>	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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<https://www.chemeo.com/cid/77-175-3/1-3-Cyclopentadiene-2-hexyl.pdf>

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