

# [2.2.2.2.2](1,2,3,4,5,6)Cyclophane

<b>Inchi:</b>	InChI=1S/C24H24/c1-2-14-17-5-3-15-13(1)16-4-6-18(14)22-10-8-20(16)23-11-12-24(22)
<b>InchiKey:</b>	BVTYOCKAKQQPEE-UHFFFAOYSA-N
<b>Formula:</b>	C24H24
<b>SMILES:</b>	C1Cc2c3c4c5c6c2CCc2c1c(c(c(c2CC6)CC5)CC4)CC3
<b>Mol. weight [g/mol]:</b>	312.45
<b>CAS:</b>	60144-50-5

## Physical Properties

Property code	Value	Unit	Source
gf	658.32	kJ/mol	Joback Method
hf	303.85	kJ/mol	Joback Method
hfus	33.73	kJ/mol	Joback Method
hvap	80.78	kJ/mol	Joback Method
ie	7.55 ± 0.02	eV	NIST Webbook
ie	7.30	eV	NIST Webbook
log10ws	-7.20		Crippen Method
logp	3.965		Crippen Method
mcvol	247.200	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
tb	895.92	K	Joback Method
tc	1148.08	K	Joback Method
tf	659.74	K	Joback Method
vc	0.978	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.08	J/molxK	895.92	Joback Method
cpg	821.25	J/molxK	937.95	Joback Method
cpg	840.67	J/molxK	979.97	Joback Method
cpg	860.69	J/molxK	1022.00	Joback Method
cpg	881.67	J/molxK	1064.03	Joback Method
cpg	903.98	J/molxK	1106.05	Joback Method
cpg	927.97	J/molxK	1148.08	Joback Method

dvisc	0.0208212	Paxs	659.74	Joback Method
dvisc	0.0205675	Paxs	699.10	Joback Method
dvisc	0.0203434	Paxs	738.47	Joback Method
dvisc	0.0201441	Paxs	777.83	Joback Method
dvisc	0.0199657	Paxs	817.19	Joback Method
dvisc	0.0198051	Paxs	856.56	Joback Method
dvisc	0.0196596	Paxs	895.92	Joback Method

## Sources

<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=C60144505&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C60144505&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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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