

# [2.2.2.2](1,2,3,4,5)Cyclophane

<b>Inchi:</b>	InChI=1S/C22H22/c1-2-14-12-16-4-3-15-11-13(1)17-5-6-18(14)22-10-9-21(17)19(15)7-8
<b>InchiKey:</b>	UVAGYNNUHRJWFD-UHFFFAOYSA-N
<b>Formula:</b>	C22H22
<b>SMILES:</b>	c1c2c3c4c5c1CCc1cc(c(c1CC5)CC4)CC3)CC2
<b>Mol. weight [g/mol]:</b>	286.41
<b>CAS:</b>	70759-58-9

## Physical Properties

Property code	Value	Unit	Source
gf	580.18	kJ/mol	Joback Method
hf	268.77	kJ/mol	Joback Method
hfus	30.16	kJ/mol	Joback Method
hvap	74.96	kJ/mol	Joback Method
ie	7.67 ± 0.02	eV	NIST Webbook
log10ws	-6.54		Crippen Method
logp	3.866		Crippen Method
mcvol	229.880	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
tb	833.06	K	Joback Method
tc	1086.08	K	Joback Method
tf	586.46	K	Joback Method
vc	0.899	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	712.40	J/mol×K	833.06	Joback Method
cpg	800.31	J/mol×K	1043.91	Joback Method
cpg	782.44	J/mol×K	1001.74	Joback Method
cpg	765.01	J/mol×K	959.57	Joback Method
cpg	747.73	J/mol×K	917.40	Joback Method
cpg	730.30	J/mol×K	875.23	Joback Method
cpg	818.93	J/mol×K	1086.08	Joback Method
dvisc	0.0057355	Paxs	833.06	Joback Method

dvisc	0.0059315	Paxs	791.96	Joback Method
dvisc	0.0061568	Paxs	750.86	Joback Method
dvisc	0.0064183	Paxs	709.76	Joback Method
dvisc	0.0067252	Paxs	668.66	Joback Method
dvisc	0.0070901	Paxs	627.56	Joback Method
dvisc	0.0075303	Paxs	586.46	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=C70759589&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C70759589&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>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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