

# [2.2.2](1,3,5)Cyclophane

<b>Other names:</b>	Tetracyclo[6.6.2.1<sup>3,13</sup>.1<sup>6,10</sup>]octadeca-1,3(17),6,8,10(18),13-h
<b>Inchi:</b>	InChI=1S/C18H18/c1-2-14-9-17-5-3-15-7-13(1)8-16(11-15)4-6-18(10-14)12-17/h7-12H,1
<b>InchiKey:</b>	KGQZPENLTBITEJ-UHFFFAOYSA-N
<b>Formula:</b>	C18H18
<b>SMILES:</b>	c1c2cc3cc1CCc1cc(cc(c1)CC3)CC2
<b>Mol. weight [g/mol]:</b>	234.34
<b>CAS:</b>	27165-88-4

## Physical Properties

Property code	Value	Unit	Source
gf	423.90	kJ/mol	Joback Method
hf	198.61	kJ/mol	Joback Method
hfus	23.03	kJ/mol	Joback Method
hvap	63.31	kJ/mol	Joback Method
ie	8.20 ± 0.05	eV	NIST Webbook
ie	7.88	eV	NIST Webbook
ie	7.70 ± 0.02	eV	NIST Webbook
log10ws	-5.22		Crippen Method
logp	3.669		Crippen Method
mcvol	195.240	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
tb	707.34	K	Joback Method
tc	963.48	K	Joback Method
tf	439.90	K	Joback Method
vc	0.744	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.83	J/mol×K	707.34	Joback Method
cpg	620.54	J/mol×K	920.79	Joback Method
cpg	606.60	J/mol×K	878.10	Joback Method
cpg	591.85	J/mol×K	835.41	Joback Method
cpg	576.10	J/mol×K	792.72	Joback Method

cpg	559.16	J/molxK	750.03	Joback Method
cpg	633.86	J/molxK	963.48	Joback Method
dvisc	0.0006163	Paxs	707.34	Joback Method
dvisc	0.0006994	Paxs	662.77	Joback Method
dvisc	0.0008084	Paxs	618.19	Joback Method
dvisc	0.0009556	Paxs	573.62	Joback Method
dvisc	0.0011619	Paxs	529.05	Joback Method
dvisc	0.0014644	Paxs	484.47	Joback Method
dvisc	0.0019344	Paxs	439.90	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=C27165884&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C27165884&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>mccvol:</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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