

# Tricyclo[8.2.2.2<sup>4,7</sup>]hexadeca-6,10,12,5,6,11,12,13,15-hexamethyl-

Other names: 2,2,5,5',5',6'-Hexamethyl-[2,2]paracyclophane  
Tricyclo[8.2.2.2

**Inchi:** InChI=1S/C22H28/c1-13-14(2)20-8-7-19(13)9-11-21-15(3)17(5)22(12-10-20)18(6)16(21)  
**InchiKey:** COWSCXIHIVAWAL-UHFFFAOYSA-N  
**Formula:** C22H28  
**SMILES:** Cc1c2ccc(c1C)CCc1c(C)c(C)c(c(C)c1C)CC2  
**Mol. weight [g/mol]:** 292.46  
**CAS:** 77897-17-7

## Physical Properties

Property code	Value	Unit	Source
gf	338.50	kJ/mol	Joback Method
hf	-29.13	kJ/mol	Joback Method
hfus	32.67	kJ/mol	Joback Method
hvap	74.81	kJ/mol	Joback Method
ie	7.00	eV	NIST Webbook
ie	7.45 ± 0.05	eV	NIST Webbook
log10ws	-7.41		Crippen Method
logp	5.421		Crippen Method
mcvol	262.460	ml/mol	McGowan Method
pc	1479.29	kPa	Joback Method
tb	811.64	K	Joback Method
tc	1044.04	K	Joback Method
tf	509.36	K	Joback Method
vc	1.002	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	784.88	J/molxK	811.64	Joback Method
cpg	869.77	J/molxK	1005.31	Joback Method
cpg	855.02	J/molxK	966.57	Joback Method
cpg	839.23	J/molxK	927.84	Joback Method
cpg	822.32	J/molxK	889.11	Joback Method

cpg	804.22	J/molxK	850.37	Joback Method
cpg	883.54	J/molxK	1044.04	Joback Method
dvisc	0.0001406	Paxs	811.64	Joback Method
dvisc	0.0001653	Paxs	761.26	Joback Method
dvisc	0.0001989	Paxs	710.88	Joback Method
dvisc	0.0002461	Paxs	660.50	Joback Method
dvisc	0.0003153	Paxs	610.12	Joback Method
dvisc	0.0004225	Paxs	559.74	Joback Method
dvisc	0.0005999	Paxs	509.36	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=C77897177&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C77897177&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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