

# Phyllocladane

<b>Inchi:</b>	InChI=1S/C20H34/c1-14-12-20-11-8-16-18(2,3)9-5-10-19(16,4)17(20)7-6-15(14)13-20/h1
<b>InchiKey:</b>	IVZWRQBQDVHDNG-VCONYVNUSA-N
<b>Formula:</b>	C20H34
<b>SMILES:</b>	CC1CC23CCC4C(C)(C)CCCC4(C)C2CCC1C3
<b>Mol. weight [g/mol]:</b>	274.48

## Physical Properties

Property code	Value	Unit	Source
gf	272.52	kJ/mol	Joback Method
hf	-204.87	kJ/mol	Joback Method
hfus	16.02	kJ/mol	Joback Method
hvap	56.07	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	6.055		Crippen Method
mcvol	249.220	ml/mol	McGowan Method
pc	1623.29	kPa	Joback Method
rinqol	2036.00		NIST Webbook
tb	687.75	K	Joback Method
tc	927.70	K	Joback Method
tf	431.82	K	Joback Method
vc	0.943	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.84	J/molxK	687.75	Joback Method
cpg	823.76	J/molxK	727.74	Joback Method
cpg	851.66	J/molxK	767.73	Joback Method
cpg	879.02	J/molxK	807.73	Joback Method
cpg	906.36	J/molxK	847.72	Joback Method
cpg	934.18	J/molxK	887.71	Joback Method
cpg	962.98	J/molxK	927.70	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R548682&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R548682&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>
<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>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>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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