

# Abietane

**Inchi:** InChI=1S/C20H36/c1-14(2)15-7-9-17-16(13-15)8-10-18-19(3,4)11-6-12-20(17,18)5/h14-19  
**InchiKey:** STIVVCHBLMGYSL-VBEQINLCSA-N  
**Formula:** C20H36  
**SMILES:** CC(C)C1CCC2C(CCC3C(C)(C)CCCC23C)C1  
**Mol. weight [g/mol]:** 276.50

## Physical Properties

Property code	Value	Unit	Source
gf	202.72	kJ/mol	Joback Method
hf	-304.35	kJ/mol	Joback Method
hfus	18.55	kJ/mol	Joback Method
hvap	57.10	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	6.301		Crippen Method
mvol	260.080	ml/mol	McGowan Method
pc	1452.35	kPa	Joback Method
rinpol	2047.00		NIST Webbook
tb	684.60	K	Joback Method
tc	912.76	K	Joback Method
tf	371.46	K	Joback Method
vc	0.974	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.11	J/mol×K	684.60	Joback Method
cpg	845.19	J/mol×K	722.63	Joback Method
cpg	872.91	J/mol×K	760.65	Joback Method
cpg	899.54	J/mol×K	798.68	Joback Method
cpg	925.39	J/mol×K	836.70	Joback Method
cpg	950.75	J/mol×K	874.73	Joback Method
cpg	975.90	J/mol×K	912.76	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=R548642&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R548642&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>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>rinpola:</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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