

# 1,3,4-Trimethyladamantane

<b>Other names:</b>	1,3,4-trimethyladamantane, trans
<b>Inchi:</b>	InChI=1S/C13H22/c1-9-11-4-10-5-12(2,7-11)8-13(9,3)6-10/h9-11H,4-8H2,1-3H3
<b>InchiKey:</b>	BWGAFPQRFLNCLN-UHFFFAOYSA-N
<b>Formula:</b>	C13H22
<b>SMILES:</b>	CC1C2CC3CC(C)(C2)CC1(C)C3
<b>Mol. weight [g/mol]:</b>	178.31

## Physical Properties

Property code	Value	Unit	Source
gf	202.33	kJ/mol	Joback Method
hf	-109.61	kJ/mol	Joback Method
hfus	11.28	kJ/mol	Joback Method
hvap	41.52	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.859		Crippen Method
mcvol	161.450	ml/mol	McGowan Method
pc	2433.84	kPa	Joback Method
rinpol	1221.00		NIST Webbook
rinpol	1221.00		NIST Webbook
tb	512.47	K	Joback Method
tc	734.57	K	Joback Method
tf	325.89	K	Joback Method
vc	0.621	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.67	J/mol×K	512.47	Joback Method
cpg	440.84	J/mol×K	549.49	Joback Method
cpg	462.14	J/mol×K	586.50	Joback Method
cpg	481.85	J/mol×K	623.52	Joback Method
cpg	500.27	J/mol×K	660.54	Joback Method
cpg	517.68	J/mol×K	697.56	Joback Method
cpg	534.37	J/mol×K	734.57	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=U214983&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U214983&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>h vap:</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>r in pol:</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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