

# 1-Methoxyadamantane

<b>Inchi:</b>	InChI=1S/C11H18O/c1-12-11-5-8-2-9(6-11)4-10(3-8)7-11/h8-10H,2-7H2,1H3
<b>InchiKey:</b>	VLBPHZFRABGLFH-UHFFFAOYSA-N
<b>Formula:</b>	C11H18O
<b>SMILES:</b>	COC12CC3CC(CC(C3)C1)C2
<b>Mol. weight [g/mol]:</b>	166.26
<b>CAS:</b>	6221-74-5

## Physical Properties

Property code	Value	Unit	Source
gf	93.69	kJ/mol	Joback Method
hf	-195.45	kJ/mol	Joback Method
hfus	12.51	kJ/mol	Joback Method
hvap	40.94	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.602		Crippen Method
mvol	139.140	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
rinpol	1178.10		NIST Webbook
tb	493.56	K	Joback Method
tc	711.44	K	Joback Method
tf	305.92	K	Joback Method
vc	0.529	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.30	J/mol×K	493.56	Joback Method
cpg	369.23	J/mol×K	529.87	Joback Method
cpg	388.59	J/mol×K	566.19	Joback Method
cpg	406.54	J/mol×K	602.50	Joback Method
cpg	423.27	J/mol×K	638.81	Joback Method
cpg	438.94	J/mol×K	675.13	Joback Method
cpg	453.73	J/mol×K	711.44	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.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>
<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=C6221745&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6221745&amp;Units=SI</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>hvp:</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>rinp:</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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