

# 1-sec-Butyladamantane

<b>Inchi:</b>	InChI=1S/C14H24/c1-3-10(2)14-7-11-4-12(8-14)6-13(5-11)9-14/h10-13H,3-9H2,1-2H3
<b>InchiKey:</b>	JEURJPFZYKZIK-UHFFFAOYSA-N
<b>Formula:</b>	C14H24
<b>SMILES:</b>	CCC(C)C12CC3CC(CC(C3)C1)C2
<b>Mol. weight [g/mol]:</b>	192.34
<b>CAS:</b>	14449-42-4

## Physical Properties

Property code	Value	Unit	Source
gf	221.51	kJ/mol	Joback Method
hf	-130.43	kJ/mol	Joback Method
hfus	15.57	kJ/mol	Joback Method
hvap	44.82	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	4.249		Crippen Method
mcvol	175.540	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
tb	539.34	K	Joback Method
tc	753.74	K	Joback Method
tf	302.50	K	Joback Method
vc	0.673	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.93	J/molxK	539.34	Joback Method
cpg	492.22	J/molxK	575.07	Joback Method
cpg	513.87	J/molxK	610.81	Joback Method
cpg	534.09	J/molxK	646.54	Joback Method
cpg	553.06	J/molxK	682.27	Joback Method
cpg	570.97	J/molxK	718.00	Joback Method
cpg	588.02	J/molxK	753.74	Joback Method

# Sources

<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=C14449424&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C14449424&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>

# 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>hvac:</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>mccol:</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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