

# Adamantane-1-carboxamide, N-(1-naphthyl)-

<b>Other names:</b>	1-Adamantanecarboxamide, N-(1-naphthyl)-
<b>Inchi:</b>	InChI=1S/C21H23NO/c23-20(21-11-14-8-15(12-21)10-16(9-14)13-21)22-19-7-3-5-17-4-1
<b>InchiKey:</b>	RJZASJFLYAWUDU-UHFFFAOYSA-N
<b>Formula:</b>	C21H23NO
<b>SMILES:</b>	O=C(Nc1cccc2ccccc12)C12CC3CC(CC(C3)C1)C2
<b>Mol. weight [g/mol]:</b>	305.41
<b>CAS:</b>	121768-37-4

## Physical Properties

Property code	Value	Unit	Source
gf	452.79	kJ/mol	Joback Method
hf	87.39	kJ/mol	Joback Method
hfus	34.59	kJ/mol	Joback Method
hvap	78.55	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	4.995		Crippen Method
mcvol	242.500	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
rinpol	2941.00		NIST Webbook
tb	854.62	K	Joback Method
tc	1108.38	K	Joback Method
tf	570.62	K	Joback Method
vc	0.926	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.41	J/molxK	854.62	Joback Method
cpg	820.21	J/molxK	896.91	Joback Method
cpg	840.91	J/molxK	939.21	Joback Method
cpg	861.91	J/molxK	981.50	Joback Method
cpg	883.58	J/molxK	1023.79	Joback Method
cpg	906.33	J/molxK	1066.09	Joback Method
cpg	930.54	J/molxK	1108.38	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=C121768374&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C121768374&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>

# 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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