

# 1-Naphthaleneacetonitrile

<b>Other names:</b>	«alpha»-Naphthylacetonitrile 1-Naphthylacetonitrile «alpha»-(1-naphthyl)acetonitrile Acetonitrile, (1-naphthyl)-
<b>Inchi:</b>	InChI=1S/C12H9N/c13-9-8-11-6-3-5-10-4-1-2-7-12(10)11/h1-7H,8H2
<b>InchiKey:</b>	OQRMWUNUKVUHQO-UHFFFAOYSA-N
<b>Formula:</b>	C12H9N
<b>SMILES:</b>	N#CCc1cccc2ccccc12
<b>Mol. weight [g/mol]:</b>	167.21
<b>CAS:</b>	132-75-2

## Physical Properties

Property code	Value	Unit	Source
gf	392.77	kJ/mol	Joback Method
hf	290.00	kJ/mol	Joback Method
hfus	19.01	kJ/mol	Joback Method
hvap	57.36	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	2.906		Crippen Method
mcvol	138.100	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
tb	626.68	K	Joback Method
tc	872.33	K	Joback Method
tf	361.63	K	Joback Method
vc	0.547	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.29	J/molxK	626.68	Joback Method
cpg	333.25	J/molxK	667.62	Joback Method
cpg	344.26	J/molxK	708.56	Joback Method
cpg	354.40	J/molxK	749.50	Joback Method
cpg	363.75	J/molxK	790.45	Joback Method

cpg	372.41	J/mol×K	831.39	Joback Method
cpg	380.46	J/mol×K	872.33	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	465.70	K	2.40	NIST Webbook

## 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.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=C132752&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C132752&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>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>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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