

# Aniline, 2,6-dicyclohexyl-

<b>Inchi:</b>	InChI=1S/C18H27N/c19-18-16(14-8-3-1-4-9-14)12-7-13-17(18)15-10-5-2-6-11-15/h7,12-
<b>InchiKey:</b>	YTDHOCZRNXHNKS-UHFFFAOYSA-N
<b>Formula:</b>	C18H27N
<b>SMILES:</b>	<chem>Nc1c(C2CCCCC2)cccc1C1CCCCC1</chem>
<b>Mol. weight [g/mol]:</b>	257.41
<b>CAS:</b>	112121-78-5

## Physical Properties

Property code	Value	Unit	Source
gf	309.18	kJ/mol	Joback Method
hf	-58.83	kJ/mol	Joback Method
hfus	24.51	kJ/mol	Joback Method
hvap	70.76	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	5.364		Crippen Method
mcvol	228.980	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
tb	759.51	K	Joback Method
tc	1018.26	K	Joback Method
tf	442.10	K	Joback Method
vc	0.831	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.59	J/molxK	759.51	Joback Method
cpg	745.38	J/molxK	802.63	Joback Method
cpg	767.11	J/molxK	845.76	Joback Method
cpg	786.88	J/molxK	888.88	Joback Method
cpg	804.79	J/molxK	932.01	Joback Method
cpg	820.93	J/molxK	975.13	Joback Method
cpg	835.42	J/molxK	1018.26	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=C112121785&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C112121785&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>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>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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