

# Nimodipine

**Other names:**

3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-,  
2-methoxyethyl 1-methylethyl ester  
BAY e 9736

Nimotop

Isopropyl 2-methoxyethyl

1,4-dihydro-2,6-dimethyl-4-(m-nitrophenyl)-3,5-pyridinedicarboxylate  
Admon

Periplum

**Inchi:** InChI=1S/C21H26N2O7/c1-12(2)30-21(25)18-14(4)22-13(3)17(20(24)29-10-9-28-5)19(18)

**InchiKey:** UIAGMCDKSXEBJQ-UHFFFAOYSA-N

**Formula:** C21H26N2O7

**SMILES:** COCCOC(=O)C1=C(C)NC(C)=C(C(=O)OC(C)C)C1c1cccc([N+](=O)[O-])c1

**Mol. weight [g/mol]:** 418.44

**CAS:** 66085-59-4

## Physical Properties

Property code	Value	Unit	Source
gf	-177.45	kJ/mol	Joback Method
hf	-727.76	kJ/mol	Joback Method
hfus	60.71	kJ/mol	Joback Method
hvap	112.62	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	2.971		Crippen Method
mvol	311.680	ml/mol	McGowan Method
pc	1501.15	kPa	Joback Method
rinpol	2840.44		NIST Webbook
rinpol	2840.44		NIST Webbook
tb	1124.28	K	Joback Method
tc	1379.69	K	Joback Method
tf	824.54	K	Joback Method
vc	1.188	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1033.16	J/molxK	1124.28	Joback Method

cpg	1038.89	J/mol×K	1166.85	Joback Method
cpg	1042.25	J/mol×K	1209.42	Joback Method
cpg	1043.21	J/mol×K	1251.98	Joback Method
cpg	1041.76	J/mol×K	1294.55	Joback Method
cpg	1037.89	J/mol×K	1337.12	Joback Method
cpg	1031.57	J/mol×K	1379.69	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=C66085594&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C66085594&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>rinpol:</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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