

# Amineptine

<b>Inchi:</b>	InChI=1S/C22H27NO2/c24-21(25)13-3-1-2-8-16-23-22-19-11-6-4-9-17(19)14-15-18-10-5
<b>InchiKey:</b>	ONNOFKFOZAJDHT-UHFFFAOYSA-N
<b>Formula:</b>	C22H27NO2
<b>SMILES:</b>	O=C(O)CCCCCNC1c2ccccc2CCc2ccccc21
<b>Mol. weight [g/mol]:</b>	337.46
<b>CAS:</b>	57574-09-1

## Physical Properties

Property code	Value	Unit	Source
gf	224.32	kJ/mol	Joback Method
hf	-185.83	kJ/mol	Joback Method
hfus	48.96	kJ/mol	Joback Method
hvap	100.22	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	4.499		Crippen Method
mcvol	279.880	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
rinpol	3085.00		NIST Webbook
rinpol	3085.00		NIST Webbook
tb	969.04	K	Joback Method
tc	1194.06	K	Joback Method
tf	596.93	K	Joback Method
vc	1.069	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	923.66	J/molxK	969.04	Joback Method
cpg	937.95	J/molxK	1006.54	Joback Method
cpg	951.43	J/molxK	1044.05	Joback Method
cpg	964.21	J/molxK	1081.55	Joback Method
cpg	976.42	J/molxK	1119.05	Joback Method
cpg	988.16	J/molxK	1156.56	Joback Method
cpg	999.55	J/molxK	1194.06	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=C57574091&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C57574091&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>hvp:</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>rinp:</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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