

# Pantanamide, N-tetrahydrofuryl-5-chloro-

Inchi:	lnChI=1S/C10H18CINO2/c11-6-2-1-5-10(13)12-8-9-4-3-7-14-9/h9H,1-8H2,(H,12,13)
InchiKey:	LGSZKARSGCPNGG-UHFFFAOYSA-N
Formula:	C10H18CINO2
SMILES:	OC(CCCCC)=NCC1CCCCO1
Mol. weight [g/mol]:	219.71

## Physical Properties

Property code	Value	Unit	Source
hf	-416.79	kJ/mol	Joback Method
hvap	67.08	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	2.531		Crippen Method
mcvol	170.560	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
rinpol	1783.00		NIST Webbook
tb	676.60	K	Joback Method
tc	877.65	K	Joback Method

## Sources

Joback Method:	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U307357&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307357&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	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

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