

# Propanamide, N,N-dinonyl-3-chloro-

<b>Inchi:</b>	InChI=1S/C21H42ClNO/c1-3-5-7-9-11-13-15-19-23(21(24)17-18-22)20-16-14-12-10-8-6-
<b>InchiKey:</b>	IXOQRAVVQUMNPF-UHFFFAOYSA-N
<b>Formula:</b>	C21H42ClNO
<b>SMILES:</b>	CCCCCCCCCN(CCCCCCCC)C(=O)CCCI
<b>Mol. weight [g/mol]:</b>	360.02

## Physical Properties

Property code	Value	Unit	Source
gf	95.87	kJ/mol	Joback Method
hf	-537.56	kJ/mol	Joback Method
hfus	58.96	kJ/mol	Joback Method
hvap	75.51	kJ/mol	Joback Method
log10ws	-7.11		Crippen Method
logp	6.945		Crippen Method
mvol	330.540	ml/mol	McGowan Method
pc	970.49	kPa	Joback Method
rinpol	2572.00		NIST Webbook
rinpol	2572.00		NIST Webbook
tb	783.62	K	Joback Method
tc	962.16	K	Joback Method
tf	438.75	K	Joback Method
vc	1.284	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1015.93	J/molxK	783.62	Joback Method
cpg	1035.59	J/molxK	813.38	Joback Method
cpg	1054.26	J/molxK	843.13	Joback Method
cpg	1071.98	J/molxK	872.89	Joback Method
cpg	1088.80	J/molxK	902.65	Joback Method
cpg	1104.77	J/molxK	932.41	Joback Method
cpg	1119.91	J/molxK	962.16	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.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=U308508&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308508&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>rinpola:</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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