

# Propane, 1-chloro-2-nitro-

<b>Other names:</b>	1-Chloro-2-nitropropane Korax Lanstan NIA 5961 Niagara 5,961 Chloronitropropan Chloronitropropane Lastan NSC 17667
<b>Inchi:</b>	InChI=1S/C3H6ClNO2/c1-3(2-4)5(6)7/h3H,2H2,1H3
<b>InchiKey:</b>	FPJNQQRSBJPGHM-UHFFFAOYSA-N
<b>Formula:</b>	C3H6ClNO2
<b>SMILES:</b>	CC(CCl)[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	123.54
<b>CAS:</b>	2425-66-3

## Physical Properties

Property code	Value	Unit	Source
gf	-4.44	kJ/mol	Joback Method
hf	-137.03	kJ/mol	Joback Method
hfus	15.56	kJ/mol	Joback Method
hvap	42.86	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	0.890		Crippen Method
mcvol	82.790	ml/mol	McGowan Method
pc	4311.22	kPa	Joback Method
tb	456.87	K	Joback Method
tc	678.61	K	Joback Method
tf	282.10	K	Joback Method
vc	0.329	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	154.66	J/mol×K	456.87	Joback Method
cpg	162.32	J/mol×K	493.83	Joback Method
cpg	169.53	J/mol×K	530.78	Joback Method
cpg	176.31	J/mol×K	567.74	Joback Method
cpg	182.68	J/mol×K	604.70	Joback Method
cpg	188.65	J/mol×K	641.66	Joback Method
cpg	194.24	J/mol×K	678.61	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=C2425663&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2425663&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>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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