

# Propyl nitrite

<b>Other names:</b>	n-C3H7ONO n-Propyl nitrite Nitrous acid, propyl ester Nitrous acid, n-propyl ester Propanol nitrite
<b>Inchi:</b>	InChI=1S/C3H7NO2/c1-2-3-6-4-5/h2-3H2,1H3
<b>InchiKey:</b>	KAOQVXHBVNKNHA-UHFFFAOYSA-N
<b>Formula:</b>	C3H7NO2
<b>SMILES:</b>	CCCON=O
<b>Mol. weight [g/mol]:</b>	89.09
<b>CAS:</b>	543-67-9

## Physical Properties

Property code	Value	Unit	Source
chl	-2030.00 ± 1.00	kJ/mol	NIST Webbook
hf	-119.00 ± 4.20	kJ/mol	NIST Webbook
hfl	-151.00	kJ/mol	NIST Webbook
hvap	32.00	kJ/mol	NIST Webbook
ie	10.34 ± 0.01	eV	NIST Webbook
log10ws	-1.35		Crippen Method
logp	1.094		Crippen Method
mcvol	70.550	ml/mol	McGowan Method
pc	4211.09	kPa	Joback Method
rinpol	486.00		NIST Webbook
rinpol	486.00		NIST Webbook
tb	330.00	K	NIST Webbook
tb	320.90 ± 0.40	K	NIST Webbook
tc	522.74	K	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	28.30	kJ/mol	260.50	NIST Webbook

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C543679&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C543679&amp;Units=SI</a>
<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>

# Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfl:</b>	Liquid phase enthalpy of formation at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>ie:</b>	Ionization energy
<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

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