

# Nitric acid, butyl ester

<b>Other names:</b>	Butyl nitrate n-C4H9ONO2
<b>Inchi:</b>	InChI=1S/C4H9NO3/c1-2-3-4-8-5(6)7/h2-4H2,1H3
<b>InchiKey:</b>	QQHZPQUHCAKSOL-UHFFFAOYSA-N
<b>Formula:</b>	C4H9NO3
<b>SMILES:</b>	CCCCO[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	119.12
<b>CAS:</b>	928-45-0

## Physical Properties

Property code	Value	Unit	Source
gf	-86.65	kJ/mol	Joback Method
hf	-268.87	kJ/mol	Joback Method
hfus	18.67	kJ/mol	Joback Method
hvap	43.60	kJ/mol	NIST Webbook
log10ws	-1.66		Crippen Method
logp	0.995		Crippen Method
mvol	90.510	ml/mol	McGowan Method
pc	3872.29	kPa	Joback Method
rinpol	801.00		NIST Webbook
tb	409.20	K	NIST Webbook
tc	670.81	K	Joback Method
tf	300.68	K	Joback Method
vc	0.359	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.87	J/molxK	465.18	Joback Method
cpg	199.97	J/molxK	499.45	Joback Method
cpg	208.69	J/molxK	533.72	Joback Method
cpg	217.04	J/molxK	567.99	Joback Method
cpg	225.02	J/molxK	602.26	Joback Method
cpg	232.62	J/molxK	636.53	Joback Method

cpg	239.85	J/mol×K	670.81	Joback Method
hvapt	44.10	kJ/mol	308.00	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.46241e+01
Coeff. B	-3.55345e+03
Coeff. C	-5.40600e+01
Temperature range (K), min.	301.92
Temperature range (K), max.	435.63

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C928450&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C928450&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</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>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>hvapt:</b>	Enthalpy of vaporization at a given temperature
<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>pvap:</b>	Vapor pressure
<b>rinpol:</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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