

# 1,2-Propanediol, 1-nitrate-

<b>Inchi:</b>	InChI=1S/C3H7NO4/c1-3(5)2-8-4(6)7/h3,5H,2H2,1H3
<b>InchiKey:</b>	OMDFJTSKBNDDRM-UHFFFAOYSA-N
<b>Formula:</b>	C3H7NO4
<b>SMILES:</b>	CC(O)CO[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	121.09

## Physical Properties

Property code	Value	Unit	Source
gf	-234.33	kJ/mol	Joback Method
hf	-405.74	kJ/mol	Joback Method
hfus	16.64	kJ/mol	Joback Method
hvap	57.56	kJ/mol	Joback Method
log10ws	-0.62		Crippen Method
logp	-0.425		Crippen Method
mcvol	82.290	ml/mol	McGowan Method
pc	5022.80	kPa	Joback Method
tb	534.04	K	Joback Method
tc	733.87	K	Joback Method
tf	335.23	K	Joback Method
vc	0.317	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.40	J/molxK	534.04	Joback Method
cpg	196.36	J/molxK	567.34	Joback Method
cpg	203.01	J/molxK	600.65	Joback Method
cpg	209.35	J/molxK	633.95	Joback Method
cpg	215.36	J/molxK	667.26	Joback Method
cpg	221.06	J/molxK	700.56	Joback Method
cpg	226.45	J/molxK	733.87	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=B6005879&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6005879&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</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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