

# 1,2,3-Propanetriol, 1-nitrate

<b>Other names:</b>	Glycerol, 1-nitrate Glycerol 1-mononitrate Glyceryl 1-mononitrate Glycerol-1-nitrat 1-MNG 1-Mononitroglycerin Glycerin 1-nitrate
<b>Inchi:</b>	InChI=1S/C3H7NO5/c5-1-3(6)2-9-4(7)8/h3,5-6H,1-2H2
<b>InchiKey:</b>	HXWLJBVVXXBZCM-UHFFFAOYSA-N
<b>Formula:</b>	C3H7NO5
<b>SMILES:</b>	O=[N+](O-)OCC(O)CO
<b>Mol. weight [g/mol]:</b>	137.09
<b>CAS:</b>	624-43-1

## Physical Properties

Property code	Value	Unit	Source
gf	-371.15	kJ/mol	Joback Method
hf	-557.97	kJ/mol	Joback Method
hfl	-577.00 ± 3.00	kJ/mol	NIST Webbook
hfus	20.73	kJ/mol	Joback Method
hvap	74.24	kJ/mol	Joback Method
log10ws	0.12		Crippen Method
logp	-1.452		Crippen Method
mcpvol	88.160	ml/mol	McGowan Method
pc	5747.92	kPa	Joback Method
tb	626.22	K	Joback Method
tc	814.77	K	Joback Method
tf	396.05	K	Joback Method
vc	0.336	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.96	J/mol×K	626.22	Joback Method

cpg	230.94	J/mol×K	657.65	Joback Method
cpg	236.61	J/mol×K	689.07	Joback Method
cpg	241.98	J/mol×K	720.50	Joback Method
cpg	247.05	J/mol×K	751.92	Joback Method
cpg	251.82	J/mol×K	783.35	Joback Method
cpg	256.30	J/mol×K	814.77	Joback Method

## Sources

<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=C624431&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C624431&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>hfl:</b>	Liquid phase 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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