

# 2-Pentanol, nitrate

<b>Other names:</b>	n-C <sub>3</sub> H <sub>7</sub> CH(CH <sub>3</sub> )NO <sub>3</sub> 2-Pentyl nitrate
<b>Inchi:</b>	InChI=1S/C <sub>5</sub> H <sub>11</sub> NO <sub>3</sub> /c1-3-4-5(2)9-6(7)8/h5H,3-4H <sub>2</sub> ,1-2H <sub>3</sub>
<b>InchiKey:</b>	RWRBSYOTDDOXKC-UHFFFAOYSA-N
<b>Formula:</b>	C <sub>5</sub> H <sub>11</sub> NO <sub>3</sub>
<b>SMILES:</b>	CCCC(C)O[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	133.15
<b>CAS:</b>	21981-48-6

## Physical Properties

Property code	Value	Unit	Source
gf	-80.67	kJ/mol	Joback Method
hf	-294.79	kJ/mol	Joback Method
hfus	17.73	kJ/mol	Joback Method
hvap	45.34	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.383		Crippen Method
mvol	104.600	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
tb	487.62	K	Joback Method
tc	695.13	K	Joback Method
tf	296.95	K	Joback Method
vc	0.409	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.11	J/mol×K	487.62	Joback Method
cpg	241.83	J/mol×K	522.21	Joback Method
cpg	252.06	J/mol×K	556.79	Joback Method
cpg	261.83	J/mol×K	591.38	Joback Method
cpg	271.12	J/mol×K	625.96	Joback Method
cpg	279.95	J/mol×K	660.55	Joback Method
cpg	288.32	J/mol×K	695.13	Joback Method

# Sources

<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=C21981486&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C21981486&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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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