

# 3-Undecyl nitrate

<b>Inchi:</b>	InChI=1S/C11H23NO3/c1-3-5-6-7-8-9-10-11(4-2)15-12(13)14/h11H,3-10H2,1-2H3
<b>InchiKey:</b>	KGEKWWIIMVPQKA-UHFFFAOYSA-N
<b>Formula:</b>	C11H23NO3
<b>SMILES:</b>	CCCCCCCCC(CC)O[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	217.31

## Physical Properties

Property code	Value	Unit	Source
gf	-30.15	kJ/mol	Joback Method
hf	-418.63	kJ/mol	Joback Method
hfus	33.27	kJ/mol	Joback Method
hvap	58.69	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	3.724		Crippen Method
mcvol	189.140	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
rinpol	1434.00		NIST Webbook
tb	624.90	K	Joback Method
tc	816.18	K	Joback Method
tf	364.57	K	Joback Method
vc	0.746	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.55	J/molxK	624.90	Joback Method
cpg	527.36	J/molxK	656.78	Joback Method
cpg	542.39	J/molxK	688.66	Joback Method
cpg	556.68	J/molxK	720.54	Joback Method
cpg	570.22	J/molxK	752.42	Joback Method
cpg	583.05	J/molxK	784.30	Joback Method
cpg	595.16	J/molxK	816.18	Joback Method

# Sources

<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=R496967&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R496967&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.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>

# 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>h vap:</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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r inpol:</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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