

# Nitrotridecane

<b>Inchi:</b>	InChI=1S/C13H27NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14(15)16/h2-13H2,1H3
<b>InchiKey:</b>	OVJFXQPAVMVKOV-UHFFFAOYSA-N
<b>Formula:</b>	C13H27NO2
<b>SMILES:</b>	CCCCCCCCCCCC[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	229.36

## Physical Properties

Property code	Value	Unit	Source
gf	94.13	kJ/mol	Joback Method
hf	-322.41	kJ/mol	Joback Method
hfus	40.79	kJ/mol	Joback Method
hvap	61.12	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.574		Crippen Method
mvol	211.450	ml/mol	McGowan Method
pc	1660.55	kPa	Joback Method
rinpol	1762.00		NIST Webbook
tb	648.68	K	Joback Method
tc	834.16	K	Joback Method
tf	379.88	K	Joback Method
vc	0.846	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	588.63	J/molxK	648.68	Joback Method
cpg	605.40	J/molxK	679.59	Joback Method
cpg	621.35	J/molxK	710.51	Joback Method
cpg	636.51	J/molxK	741.42	Joback Method
cpg	650.90	J/molxK	772.34	Joback Method
cpg	664.57	J/molxK	803.25	Joback Method
cpg	677.53	J/molxK	834.16	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=R518691&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R518691&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>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical 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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