

# Norephedrine, N-propyloxycarbonyl-

<b>Other names:</b>	Norephedrine, N-propoxycarbonyl
<b>Inchi:</b>	InChI=1S/C13H19NO3/c1-3-9-17-13(16)14-10(2)12(15)11-7-5-4-6-8-11/h4-8,10,12,15H,3
<b>InchiKey:</b>	VIZIBJLJLBAQN-UHFFFAOYSA-N
<b>Formula:</b>	C13H19NO3
<b>SMILES:</b>	CCCOC(=O)NC(C)C(O)c1ccccc1
<b>Mol. weight [g/mol]:</b>	237.29

## Physical Properties

Property code	Value	Unit	Source
gf	-115.24	kJ/mol	Joback Method
hf	-429.24	kJ/mol	Joback Method
hfus	28.39	kJ/mol	Joback Method
hvap	78.30	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.245		Crippen Method
mvol	193.560	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
tb	741.28	K	Joback Method
tc	940.82	K	Joback Method
tf	418.33	K	Joback Method
vc	0.722	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.78	J/molxK	741.28	Joback Method
cpg	568.73	J/molxK	774.54	Joback Method
cpg	580.83	J/molxK	807.79	Joback Method
cpg	592.11	J/molxK	841.05	Joback Method
cpg	602.61	J/molxK	874.31	Joback Method
cpg	612.35	J/molxK	907.57	Joback Method
cpg	621.35	J/molxK	940.82	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=U314785&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U314785&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>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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