

# Propanamide, 2-methyl-N-ethyl-N-dodecyl-

<b>Inchi:</b>	InChI=1S/C18H37NO/c1-5-7-8-9-10-11-12-13-14-15-16-19(6-2)18(20)17(3)4/h17H,5-16H
<b>InchiKey:</b>	AZSUCJTUAVOEAP-UHFFFAOYSA-N
<b>Formula:</b>	C18H37NO
<b>SMILES:</b>	CCCCCCCCCCCCN(CC)C(=O)C(C)C
<b>Mol. weight [g/mol]:</b>	283.49

## Physical Properties

Property code	Value	Unit	Source
gf	80.10	kJ/mol	Joback Method
hf	-465.18	kJ/mol	Joback Method
hfus	43.47	kJ/mol	Joback Method
hvap	64.06	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	5.412		Crippen Method
mcvol	276.030	ml/mol	McGowan Method
pc	1208.15	kPa	Joback Method
rinpol	2449.00		NIST Webbook
rinpol	2449.00		NIST Webbook
tb	677.11	K	Joback Method
tc	845.94	K	Joback Method
tf	360.02	K	Joback Method
vc	1.062	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	800.05	J/mol×K	677.11	Joback Method
cpg	819.51	J/mol×K	705.25	Joback Method
cpg	838.08	J/mol×K	733.39	Joback Method
cpg	855.79	J/mol×K	761.53	Joback Method
cpg	872.66	J/mol×K	789.66	Joback Method
cpg	888.73	J/mol×K	817.80	Joback Method
cpg	904.04	J/mol×K	845.94	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<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=U415350&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U415350&amp;Units=SI</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>rinpola:</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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