

# Propanamide, N-(1-naphthyl)-3-chloro-

<b>Inchi:</b>	InChI=1S/C13H12ClNO/c14-9-8-13(16)15-12-7-3-5-10-4-1-2-6-11(10)12/h1-7H,8-9H2,(H
<b>InchiKey:</b>	ISEAPHXDUWABSS-UHFFFAOYSA-N
<b>Formula:</b>	C13H12ClNO
<b>SMILES:</b>	O=C(CCCl)Nc1cccc2ccccc12
<b>Mol. weight [g/mol]:</b>	233.69

## Physical Properties

Property code	Value	Unit	Source
gf	216.55	kJ/mol	Joback Method
hf	29.63	kJ/mol	Joback Method
hfus	30.99	kJ/mol	Joback Method
hvap	66.68	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.407		Crippen Method
mvol	174.600	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
rinpol	2158.00		NIST Webbook
rinpol	2158.00		NIST Webbook
tb	688.95	K	Joback Method
tc	923.73	K	Joback Method
tf	440.42	K	Joback Method
vc	0.667	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.45	J/mol×K	688.95	Joback Method
cpg	446.13	J/mol×K	728.08	Joback Method
cpg	457.84	J/mol×K	767.21	Joback Method
cpg	468.64	J/mol×K	806.34	Joback Method
cpg	478.64	J/mol×K	845.47	Joback Method
cpg	487.91	J/mol×K	884.60	Joback Method
cpg	496.54	J/mol×K	923.73	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=U307232&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307232&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>hvp:</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>rlnol:</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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