

# Propanamide, 3-phenyl-N-ethyl-N-isobutyl-

<b>Inchi:</b>	InChI=1S/C15H23NO/c1-4-16(12-13(2)3)15(17)11-10-14-8-6-5-7-9-14/h5-9,13H,4,10-12
<b>InchiKey:</b>	LEOSSYMCQYJDIB-UHFFFAOYSA-N
<b>Formula:</b>	C15H23NO
<b>SMILES:</b>	CCN(CC(C)C)C(=O)CCc1ccccc1
<b>Mol. weight [g/mol]:</b>	233.35

## Physical Properties

Property code	Value	Unit	Source
gf	167.25	kJ/mol	Joback Method
hf	-166.73	kJ/mol	Joback Method
hfus	29.74	kJ/mol	Joback Method
hvap	59.66	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	3.124		Crippen Method
mcvol	210.000	ml/mol	McGowan Method
pc	1961.34	kPa	Joback Method
tb	635.15	K	Joback Method
tc	835.55	K	Joback Method
tf	352.63	K	Joback Method
vc	0.785	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.61	J/molxK	635.15	Joback Method
cpg	575.42	J/molxK	668.55	Joback Method
cpg	592.16	J/molxK	701.95	Joback Method
cpg	607.88	J/molxK	735.35	Joback Method
cpg	622.63	J/molxK	768.75	Joback Method
cpg	636.46	J/molxK	802.15	Joback Method
cpg	649.43	J/molxK	835.55	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U415391&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U415391&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

# 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>mccvol:</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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