

# Pentanamide, N-heptyl-N-octyl-

<b>Inchi:</b>	InChI=1S/C20H41NO/c1-4-7-10-12-14-16-19-21(20(22)17-9-6-3)18-15-13-11-8-5-2/h4-1
<b>InchiKey:</b>	ZFBQPSOZW SCKHA-UHFFFAOYSA-N
<b>Formula:</b>	C20H41NO
<b>SMILES:</b>	CCCCCCCCN(CCCCCC)C(=O)CCCC
<b>Mol. weight [g/mol]:</b>	311.55

## Physical Properties

Property code	Value	Unit	Source
gf	99.38	kJ/mol	Joback Method
hf	-501.18	kJ/mol	Joback Method
hfus	52.18	kJ/mol	Joback Method
hvap	68.90	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	6.336		Crippen Method
mvol	304.210	ml/mol	McGowan Method
pc	1056.20	kPa	Joback Method
rinpol	2211.00		NIST Webbook
tb	723.31	K	Joback Method
tc	893.05	K	Joback Method
tf	397.56	K	Joback Method
vc	1.179	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.49	J/molxK	723.31	Joback Method
cpg	938.52	J/molxK	751.60	Joback Method
cpg	957.61	J/molxK	779.89	Joback Method
cpg	975.81	J/molxK	808.18	Joback Method
cpg	993.15	J/molxK	836.47	Joback Method
cpg	1009.65	J/molxK	864.76	Joback Method
cpg	1025.37	J/molxK	893.05	Joback Method

# Sources

<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>
<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=U308184&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308184&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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