

# Hexadecylamine, N,N-di(allyl)-

<b>Inchi:</b>	InChI=1S/C22H43N/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-22-23(20-5-2)21-6-3/h5-
<b>InchiKey:</b>	FDVMDNBDNHHXAO-UHFFFAOYSA-N
<b>Formula:</b>	C22H43N
<b>SMILES:</b>	C=CCN(CC=C)CCCCCCCCCCCCCCCCCC
<b>Mol. weight [g/mol]:</b>	321.58

## Physical Properties

Property code	Value	Unit	Source
gf	420.82	kJ/mol	Joback Method
hf	-179.02	kJ/mol	Joback Method
hfus	53.20	kJ/mol	Joback Method
hvap	65.27	kJ/mol	Joback Method
log10ws	-7.31		Crippen Method
logp	7.142		Crippen Method
mcvol	322.220	ml/mol	McGowan Method
pc	947.91	kPa	Joback Method
rinsol	1249.00		NIST Webbook
tb	708.56	K	Joback Method
tc	874.64	K	Joback Method
tf	366.65	K	Joback Method
vc	1.248	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.66	J/mol×K	708.56	Joback Method
cpg	976.68	J/mol×K	736.24	Joback Method
cpg	996.76	J/mol×K	763.92	Joback Method
cpg	1015.93	J/mol×K	791.60	Joback Method
cpg	1034.23	J/mol×K	819.28	Joback Method
cpg	1051.71	J/mol×K	846.96	Joback Method
cpg	1068.41	J/mol×K	874.64	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=U416179&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416179&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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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