

# Octadecylamine, N,N-diethyl

<b>Inchi:</b>	InChI=1S/C22H47N/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23(5-2)6-3/h4-
<b>InchiKey:</b>	MNOIOAHRVYPSPE-UHFFFAOYSA-N
<b>Formula:</b>	C22H47N
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCCN(CC)CC
<b>Mol. weight [g/mol]:</b>	325.62

## Physical Properties

Property code	Value	Unit	Source
gf	245.14	kJ/mol	Joback Method
hf	-429.88	kJ/mol	Joback Method
hfus	55.76	kJ/mol	Joback Method
hvap	66.61	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	7.590		Crippen Method
mvol	330.820	ml/mol	McGowan Method
pc	900.72	kPa	Joback Method
rinpol	2241.00		NIST Webbook
tb	715.20	K	Joback Method
tc	880.05	K	Joback Method
tf	370.17	K	Joback Method
vc	1.286	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1006.10	J/mol×K	715.20	Joback Method
cpg	1028.15	J/mol×K	742.67	Joback Method
cpg	1049.24	J/mol×K	770.15	Joback Method
cpg	1069.38	J/mol×K	797.62	Joback Method
cpg	1088.62	J/mol×K	825.10	Joback Method
cpg	1107.00	J/mol×K	852.57	Joback Method
cpg	1124.55	J/mol×K	880.05	Joback Method

# Sources

<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=R543503&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R543503&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.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>

# 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>h vap:</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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r inpol:</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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