

# N,N'-Di-n-hexylsebacamide

<b>Inchi:</b>	InChI=1S/C22H44N2O2/c1-3-5-7-15-19-23-21(25)17-13-11-9-10-12-14-18-22(26)24-20-
<b>InchiKey:</b>	ANLFZJDBTDDXJA-UHFFFAOYSA-N
<b>Formula:</b>	C22H44N2O2
<b>SMILES:</b>	CCCCCNC(=O)CCCCCCCC(=O)NCCCCC
<b>Mol. weight [g/mol]:</b>	368.60
<b>CAS:</b>	31827-03-9

## Physical Properties

Property code	Value	Unit	Source
gf	55.30	kJ/mol	Joback Method
hf	-615.63	kJ/mol	Joback Method
hfus	66.13	kJ/mol	Joback Method
hvap	90.93	kJ/mol	Joback Method
log10ws	-6.96		Crippen Method
logp	5.500		Crippen Method
mcvol	343.940	ml/mol	McGowan Method
pc	990.13	kPa	Joback Method
tb	910.84	K	Joback Method
tc	1115.72	K	Joback Method
tf	415.00 ± 1.00	K	NIST Webbook
vc	1.349	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1195.82	J/molxK	979.13	Joback Method
cpg	1212.51	J/molxK	1013.28	Joback Method
cpg	1228.12	J/molxK	1047.43	Joback Method
cpg	1242.72	J/molxK	1081.57	Joback Method
cpg	1158.95	J/molxK	910.84	Joback Method
cpg	1177.98	J/molxK	944.99	Joback Method
cpg	1256.36	J/molxK	1115.72	Joback Method
cps	1064.10	J/molxK	408.00	NIST Webbook
hfust	53.56	kJ/mol	415.00	NIST Webbook

hfust	53.68	kJ/mol	415.00	NIST Webbook
sfust	129.30	J/mol×K	415.00	NIST Webbook

## Sources

<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=C31827039&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C31827039&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>cps:</b>	Solid phase 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>hfust:</b>	Enthalpy of fusion at a given temperature
<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>sfust:</b>	Entropy of fusion at a given temperature
<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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