

# Didodecylamine, n-butyl-

<b>Inchi:</b>	InChI=1S/C28H59N/c1-4-7-10-12-14-16-18-20-22-24-27-29(26-9-6-3)28-25-23-21-19-17
<b>InchiKey:</b>	AAYBEEVEVAWXAI-UHFFFAOYSA-N
<b>Formula:</b>	C28H59N
<b>SMILES:</b>	CCCCCCCCCCCCN(CCCC)CCCCCCCCCCCC
<b>Mol. weight [g/mol]:</b>	409.77
<b>CAS:</b>	52770-72-6

## Physical Properties

Property code	Value	Unit	Source
gf	295.66	kJ/mol	Joback Method
hf	-553.72	kJ/mol	Joback Method
hfus	71.30	kJ/mol	Joback Method
hvap	79.96	kJ/mol	Joback Method
log10ws	-10.11		Crippen Method
logp	9.930		Crippen Method
mcvol	415.360	ml/mol	McGowan Method
pc	654.77	kPa	Joback Method
tb	852.48	K	Joback Method
tc	1046.78	K	Joback Method
tf	437.79	K	Joback Method
vc	1.621	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1394.43	J/molxK	852.48	Joback Method
cpg	1420.37	J/molxK	884.86	Joback Method
cpg	1444.92	J/molxK	917.25	Joback Method
cpg	1468.17	J/molxK	949.63	Joback Method
cpg	1490.18	J/molxK	982.01	Joback Method
cpg	1511.04	J/molxK	1014.39	Joback Method
cpg	1530.80	J/molxK	1046.78	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=C52770726&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C52770726&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>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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