

# 20,24-Dimethyl-nonacosyl cyanide

**Inchi:** InChI=1S/C32H63N/c1-4-5-22-26-31(2)28-25-29-32(3)27-23-20-18-16-14-12-10-8-6-7-9-  
**InchiKey:** IOLJPKTXWZHTR-UHFFFAOYSA-N  
**Formula:** C32H63N  
**SMILES:** CCCCC(C)CCCC(C)CCCCCCCCCCCCCCCCCCCCC#N  
**Mol. weight [g/mol]:** 461.85

## Physical Properties

Property code	Value	Unit	Source
gf	346.86	kJ/mol	Joback Method
hf	-549.49	kJ/mol	Joback Method
hfus	73.10	kJ/mol	Joback Method
hvap	96.53	kJ/mol	Joback Method
log10ws	-12.60		Crippen Method
logp	11.945		Crippen Method
mcvol	463.120	ml/mol	McGowan Method
pc	541.08	kPa	Joback Method
rinpol	3431.00		NIST Webbook
tb	1032.76	K	Joback Method
tc	1292.63	K	Joback Method
tf	485.39	K	Joback Method
vc	1.841	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1669.85	J/molxK	1032.76	Joback Method
cpg	1697.14	J/molxK	1076.07	Joback Method
cpg	1722.46	J/molxK	1119.38	Joback Method
cpg	1746.01	J/molxK	1162.70	Joback Method
cpg	1767.94	J/molxK	1206.01	Joback Method
cpg	1788.44	J/molxK	1249.32	Joback Method
cpg	1807.69	J/molxK	1292.63	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=R202569&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R202569&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>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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