

# 22,26-Dimethyl-hentriacontyl cyanide

**Inchi:** InChI=1S/C34H67N/c1-4-5-24-28-33(2)30-27-31-34(3)29-25-22-20-18-16-14-12-10-8-6-7  
**InchiKey:** FNRZJMMLJPBTGZ-UHFFFAOYSA-N  
**Formula:** C34H67N  
**SMILES:** CCCCC(C)CCCC(C)CCCCCCCCCCCCCCCCCCCCC#N  
**Mol. weight [g/mol]:** 489.90

## Physical Properties

Property code	Value	Unit	Source
gf	363.70	kJ/mol	Joback Method
hf	-590.77	kJ/mol	Joback Method
hfus	78.28	kJ/mol	Joback Method
hvap	100.98	kJ/mol	Joback Method
log10ws	-13.44		Crippen Method
logp	12.725		Crippen Method
mvol	491.300	ml/mol	McGowan Method
pc	495.81	kPa	Joback Method
rinpol	3624.00		NIST Webbook
tb	1078.52	K	Joback Method
tc	1369.67	K	Joback Method
tf	507.93	K	Joback Method
vc	1.954	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1805.02	J/mol×K	1078.52	Joback Method
cpg	1834.94	J/mol×K	1127.05	Joback Method
cpg	1862.53	J/mol×K	1175.57	Joback Method
cpg	1888.05	J/mol×K	1224.10	Joback Method
cpg	1911.77	J/mol×K	1272.62	Joback Method
cpg	1933.94	J/mol×K	1321.15	Joback Method
cpg	1954.84	J/mol×K	1369.67	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=R202658&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R202658&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>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>rinpola:</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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