

# 18,22,26-Trimethyl-nonacosyl cyanide

**Inchi:** InChI=1S/C33H65N/c1-5-24-31(2)26-22-28-33(4)29-23-27-32(3)25-20-18-16-14-12-10-8  
**InchiKey:** XMTRGLQNTSHQKR-UHFFFAOYSA-N  
**Formula:** C33H65N  
**SMILES:** CCCC(C)CCCC(C)CCCC(C)CCCCCCCCCCCCCCCCCCC#N  
**Mol. weight [g/mol]:** 475.88

## Physical Properties

Property code	Value	Unit	Source
gf	352.84	kJ/mol	Joback Method
hf	-575.41	kJ/mol	Joback Method
hfus	72.16	kJ/mol	Joback Method
hvap	98.37	kJ/mol	Joback Method
log10ws	-12.78		Crippen Method
logp	12.191		Crippen Method
mvol	477.210	ml/mol	McGowan Method
pc	519.59	kPa	Joback Method
rinpol	3466.00		NIST Webbook
rinpol	3466.00		NIST Webbook
tb	1055.20	K	Joback Method
tc	1326.09	K	Joback Method
tf	481.66	K	Joback Method
vc	1.891	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1737.40	J/molxK	1055.20	Joback Method
cpg	1765.47	J/molxK	1100.35	Joback Method
cpg	1791.43	J/molxK	1145.50	Joback Method
cpg	1815.49	J/molxK	1190.64	Joback Method
cpg	1837.86	J/molxK	1235.79	Joback Method
cpg	1858.74	J/molxK	1280.94	Joback Method
cpg	1878.34	J/molxK	1326.09	Joback Method

# 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=R202410&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R202410&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>hvp:</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>rinp:</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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