

# 20-Methyl-hentriacontyl cyanide

**Inchi:** InChI=1S/C33H65N/c1-3-4-5-6-7-18-21-24-27-30-33(2)31-28-25-22-19-16-14-12-10-8-9-  
**InchiKey:** IUPJCSSBxBHZBM-UHFFFAOYSA-N  
**Formula:** C33H65N  
**SMILES:** CCCCCCCCCC(C)CCCCCCCCCCCCCCCCCCCC#N  
**Mol. weight [g/mol]:** 475.88

## Physical Properties

Property code	Value	Unit	Source
gf	357.72	kJ/mol	Joback Method
hf	-564.85	kJ/mol	Joback Method
hfus	79.21	kJ/mol	Joback Method
hvap	99.14	kJ/mol	Joback Method
log10ws	-13.26		Crippen Method
logp	12.479		Crippen Method
mvol	477.210	ml/mol	McGowan Method
pc	515.83	kPa	Joback Method
rinpol	3589.00		NIST Webbook
rinpol	3589.00		NIST Webbook
tb	1056.08	K	Joback Method
tc	1334.66	K	Joback Method
tf	511.66	K	Joback Method
vc	1.903	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1737.14	J/mol×K	1056.08	Joback Method
cpg	1766.19	J/mol×K	1102.51	Joback Method
cpg	1793.05	J/mol×K	1148.94	Joback Method
cpg	1817.97	J/mol×K	1195.37	Joback Method
cpg	1841.16	J/mol×K	1241.80	Joback Method
cpg	1862.86	J/mol×K	1288.23	Joback Method
cpg	1883.28	J/mol×K	1334.66	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R202623&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R202623&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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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