

# 20,24,28-Trimethyl-tritriacontyl cyanide

**Inchi:** InChI=1S/C37H73N/c1-5-6-23-28-35(2)30-26-32-37(4)33-27-31-36(3)29-24-21-19-17-15  
**InchiKey:** WZJJCHKEVMDZAX-UHFFFAOYSA-N  
**Formula:** C37H73N  
**SMILES:** CCCCC(C)CCCC(C)CCCC(C)CCCCCCCCCCCCCCCCCCCC#N  
**Mol. weight [g/mol]:** 531.98

## Physical Properties

Property code	Value	Unit	Source
gf	386.52	kJ/mol	Joback Method
hf	-657.97	kJ/mol	Joback Method
hfus	82.52	kJ/mol	Joback Method
hvap	107.27	kJ/mol	Joback Method
log10ws	-14.45		Crippen Method
logp	13.751		Crippen Method
mvol	533.570	ml/mol	McGowan Method
pc	439.32	kPa	Joback Method
rinpol	3839.00		NIST Webbook
rinpol	3839.00		NIST Webbook
tb	1146.72	K	Joback Method
tc	1493.02	K	Joback Method
tf	526.74	K	Joback Method
vc	2.115	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2009.86	J/molxK	1146.72	Joback Method
cpg	2044.04	J/molxK	1204.44	Joback Method
cpg	2075.26	J/molxK	1262.15	Joback Method
cpg	2104.00	J/molxK	1319.87	Joback Method
cpg	2130.74	J/molxK	1377.59	Joback Method
cpg	2155.97	J/molxK	1435.30	Joback Method
cpg	2180.18	J/molxK	1493.02	Joback Method

# Sources

<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=R202534&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R202534&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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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