

# 16,20,24-Trimethyl-tritriacontyl cyanide

**Inchi:** InChI=1S/C38H75N/c1-5-6-7-8-9-18-21-24-29-36(2)31-27-33-38(4)34-28-32-37(3)30-25-38  
**InchiKey:** PEXVTANURKOU DL-UHFFFAOYSA-N  
**Formula:** C38H75N  
**SMILES:** CCCCCCCCCC(C)CCCC(C)CCCC(C)CCCCCCCCCCCCCCCCC#N  
**Mol. weight [g/mol]:** 546.01

## Physical Properties

Property code	Value	Unit	Source
gf	394.94	kJ/mol	Joback Method
hf	-678.61	kJ/mol	Joback Method
hfus	85.11	kJ/mol	Joback Method
hvap	109.50	kJ/mol	Joback Method
log10ws	-14.87		Crippen Method
logp	14.141		Crippen Method
mvol	547.660	ml/mol	McGowan Method
pc	422.16	kPa	Joback Method
rinpol	3824.00		NIST Webbook
rinpol	3824.00		NIST Webbook
tb	1169.60	K	Joback Method
tc	1540.26	K	Joback Method
tf	538.01	K	Joback Method
vc	2.171	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2078.62	J/mol×K	1169.60	Joback Method
cpg	2114.76	J/mol×K	1231.38	Joback Method
cpg	2147.68	J/mol×K	1293.15	Joback Method
cpg	2177.99	J/mol×K	1354.93	Joback Method
cpg	2206.31	J/mol×K	1416.71	Joback Method
cpg	2233.25	J/mol×K	1478.49	Joback Method
cpg	2259.42	J/mol×K	1540.26	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=R202336&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R202336&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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r in pol:</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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