

# 16,20,24,28-Tetramethyl-hentriacontyl cyanide

**Inchi:** InChI=1S/C37H73N/c1-6-7-25-34(2)27-22-29-36(4)31-24-32-37(5)30-23-28-35(3)26-20-1  
**InchiKey:** KVICQHLMNBUBMM-UHFFFAOYSA-N  
**Formula:** C37H73N  
**SMILES:** CCCCC(C)CCCC(C)CCCC(C)CCCC(C)CCCCCCCCCCCCCCCCC#N  
**Mol. weight [g/mol]:** 531.98

## Physical Properties

Property code	Value	Unit	Source
gf	384.08	kJ/mol	Joback Method
hf	-663.25	kJ/mol	Joback Method
hfus	79.00	kJ/mol	Joback Method
hvap	106.88	kJ/mol	Joback Method
log10ws	-14.21		Crippen Method
logp	13.607		Crippen Method
mcvol	533.570	ml/mol	McGowan Method
pc	440.80	kPa	Joback Method
rinpol	3681.00		NIST Webbook
rinpol	3681.00		NIST Webbook
tb	1146.28	K	Joback Method
tc	1486.31	K	Joback Method
tf	511.74	K	Joback Method
vc	2.110	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2009.73	J/mol×K	1146.28	Joback Method
cpg	2043.14	J/mol×K	1202.95	Joback Method
cpg	2073.65	J/mol×K	1259.62	Joback Method
cpg	2101.71	J/mol×K	1316.30	Joback Method
cpg	2127.78	J/mol×K	1372.97	Joback Method
cpg	2152.33	J/mol×K	1429.64	Joback Method
cpg	2175.81	J/mol×K	1486.31	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R202272&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R202272&amp;Units=SI</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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