

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

<b>Inchi:</b>	InChI=1S/C39H77N/c1-6-7-8-21-27-36(2)29-24-31-38(4)33-26-34-39(5)32-25-30-37(3)28
<b>InchiKey:</b>	KNMUUJSPBRLSGP-UHFFFAOYSA-N
<b>Formula:</b>	C39H77N
<b>SMILES:</b>	CCCCCCC(C)CCCC(C)CCCC(C)CCCC(C)CCCCCCCCCCCCCCCCC#N
<b>Mol. weight [g/mol]:</b>	560.04

## Physical Properties

Property code	Value	Unit	Source
gf	400.92	kJ/mol	Joback Method
hf	-704.53	kJ/mol	Joback Method
hfus	84.18	kJ/mol	Joback Method
hvap	111.33	kJ/mol	Joback Method
log10ws	-15.05		Crippen Method
logp	14.387		Crippen Method
mvol	561.750	ml/mol	McGowan Method
pc	407.30	kPa	Joback Method
rinpol	3855.00		NIST Webbook
rinpol	3855.00		NIST Webbook
tb	1192.04	K	Joback Method
tc	1581.68	K	Joback Method
tf	534.28	K	Joback Method
vc	2.221	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2147.33	J/mol×K	1192.04	Joback Method
cpg	2184.65	J/mol×K	1256.98	Joback Method
cpg	2218.58	J/mol×K	1321.92	Joback Method
cpg	2249.83	J/mol×K	1386.86	Joback Method
cpg	2279.15	J/mol×K	1451.80	Joback Method
cpg	2307.25	J/mol×K	1516.74	Joback Method
cpg	2334.89	J/mol×K	1581.68	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.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=R202292&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R202292&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>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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