

# 18,22,26-Trimethyl-triacontyl cyanide

<b>Inchi:</b>	InChI=1S/C34H67N/c1-5-6-25-32(2)27-23-29-34(4)30-24-28-33(3)26-21-19-17-15-13-11
<b>InchiKey:</b>	SDUWOTAQXBQQFV-UHFFFAOYSA-N
<b>Formula:</b>	C34H67N
<b>SMILES:</b>	CCCC(C)CCCC(C)CCCC(C)CCCCCCCCCCCCCCCCCCC#N
<b>Mol. weight [g/mol]:</b>	489.90

## Physical Properties

Property code	Value	Unit	Source
gf	361.26	kJ/mol	Joback Method
hf	-596.05	kJ/mol	Joback Method
hfus	74.75	kJ/mol	Joback Method
hvap	100.59	kJ/mol	Joback Method
log10ws	-13.20		Crippen Method
logp	12.581		Crippen Method
mvol	491.300	ml/mol	McGowan Method
pc	497.58	kPa	Joback Method
rinpol	3549.00		NIST Webbook
rinpol	3549.00		NIST Webbook
tb	1078.08	K	Joback Method
tc	1364.87	K	Joback Method
tf	492.93	K	Joback Method
vc	1.948	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1805.09	J/mol×K	1078.08	Joback Method
cpg	1834.47	J/mol×K	1125.88	Joback Method
cpg	1861.55	J/mol×K	1173.68	Joback Method
cpg	1886.59	J/mol×K	1221.47	Joback Method
cpg	1909.84	J/mol×K	1269.27	Joback Method
cpg	1931.55	J/mol×K	1317.07	Joback Method
cpg	1951.98	J/mol×K	1364.87	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=R202430&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R202430&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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