

# cis-3,6,9,12,15-heneicosapentaene

Inchi:	InChI=1S/C21H34/c1-3-5-7-9-11-13-15-17-19-21-20-18-16-14-12-10-8-6-4-2/h5,7,11-14,
InchiKey:	WVVMNHZOU MNOLT-LOYOHVQTSA-N
Formula:	C21H34
SMILES:	CCC=CCC=CCC=CCC=CCC=CCCCC
Mol. weight [g/mol]:	286.49

## Physical Properties

Property code	Value	Unit	Source
gf	527.04	kJ/mol	Joback Method
hf	109.33	kJ/mol	Joback Method
hfus	51.16	kJ/mol	Joback Method
hvap	62.13	kJ/mol	Joback Method
log10ws	-7.88		Crippen Method
logp	7.318		Crippen Method
mcvol	285.250	ml/mol	McGowan Method
pc	1130.62	kPa	Joback Method
rinpol	2008.00		NIST Webbook
rinpol	2008.00		NIST Webbook
ripol	2318.00		NIST Webbook
ripol	2318.00		NIST Webbook
tb	700.68	K	Joback Method
tc	883.89	K	Joback Method
tf	301.03	K	Joback Method
vc	1.111	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.26	J/molxK	700.68	Joback Method
cpg	811.46	J/molxK	731.22	Joback Method
cpg	829.74	J/molxK	761.75	Joback Method
cpg	847.17	J/molxK	792.29	Joback Method
cpg	863.85	J/molxK	822.82	Joback Method
cpg	879.86	J/molxK	853.36	Joback Method

cpg	895.26	J/mol×K	883.89	Joback Method
dvisc	0.0025087	Paxs	301.03	Joback Method
dvisc	0.0006800	Paxs	367.64	Joback Method
dvisc	0.0002751	Paxs	434.25	Joback Method
dvisc	0.0001416	Paxs	500.86	Joback Method
dvisc	0.0000852	Paxs	567.46	Joback Method
dvisc	0.0000570	Paxs	634.07	Joback Method
dvisc	0.0000412	Paxs	700.68	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R485695&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R485695&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	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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