

# 13,17,21-trimethylnonatriacontane

<b>Inchi:</b>	InChI=1S/C42H86/c1-6-8-10-12-14-16-18-19-20-21-22-23-25-27-29-31-35-41(4)37-33-39
<b>InchiKey:</b>	RQSDFWTXQZBTCH-UHFFFAOYSA-N
<b>Formula:</b>	C42H86
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CCCC(C)CCCCCCCCCCCC
<b>Mol. weight [g/mol]:</b>	591.13

## Physical Properties

Property code	Value	Unit	Source
gf	295.44	kJ/mol	Joback Method
hf	-926.05	kJ/mol	Joback Method
hfus	93.97	kJ/mol	Joback Method
hvap	107.92	kJ/mol	Joback Method
log10ws	-16.68		Crippen Method
logp	16.198		Crippen Method
mcvol	602.640	ml/mol	McGowan Method
pc	366.15	kPa	Joback Method
rinpol	3980.00		NIST Webbook
rinpol	3980.00		NIST Webbook
rinpol	3977.00		NIST Webbook
rinpol	3980.00		NIST Webbook
tb	1159.04	K	Joback Method
tc	1569.41	K	Joback Method
tf	518.10	K	Joback Method
vc	2.369	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2317.43	J/molxK	1159.04	Joback Method
cpg	2363.53	J/molxK	1227.44	Joback Method
cpg	2405.17	J/molxK	1295.83	Joback Method
cpg	2443.29	J/molxK	1364.23	Joback Method
cpg	2478.81	J/molxK	1432.62	Joback Method
cpg	2512.67	J/molxK	1501.02	Joback Method

cpg	2545.81	J/molxK	1569.41	Joback Method
dvisc	0.0002834	Paxs	518.10	Joback Method
dvisc	0.0000668	Paxs	624.92	Joback Method
dvisc	0.0000240	Paxs	731.75	Joback Method
dvisc	0.0000112	Paxs	838.57	Joback Method
dvisc	0.0000062	Paxs	945.39	Joback Method
dvisc	0.0000039	Paxs	1052.22	Joback Method
dvisc	0.0000026	Paxs	1159.04	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=R272018&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R272018&amp;Units=SI</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>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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