

# (S)-13-methyl-nonacosane

**Inchi:** InChI=1S/C30H62/c1-4-6-8-10-12-14-16-17-18-19-21-23-25-27-29-30(3)28-26-24-22-20-19-17-15-13-11-9-7-5-3-1  
**InchiKey:** LKHFDNVPHQIRIMQ-SSEXGKCCSA-N  
**Formula:** C30H62  
**SMILES:** CCCCCCCCCCCCCCCCC(C)CCCCCCCCCCCC  
**Mol. weight [g/mol]:** 422.81

## Physical Properties

Property code	Value	Unit	Source
gf	199.28	kJ/mol	Joback Method
hf	-667.81	kJ/mol	Joback Method
hfus	69.93	kJ/mol	Joback Method
hvap	81.99	kJ/mol	Joback Method
log10ws	-12.14		Crippen Method
logp	11.805		Crippen Method
mvol	433.560	ml/mol	McGowan Method
pc	597.80	kPa	Joback Method
rinpol	2955.00		NIST Webbook
rinpol	2955.00		NIST Webbook
tb	885.36	K	Joback Method
tc	1090.03	K	Joback Method
tf	412.86	K	Joback Method
vc	1.710	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1482.38	J/molxK	885.36	Joback Method
cpg	1603.48	J/molxK	1055.92	Joback Method
cpg	1582.00	J/molxK	1021.80	Joback Method
cpg	1559.23	J/molxK	987.69	Joback Method
cpg	1535.09	J/molxK	953.58	Joback Method
cpg	1509.50	J/molxK	919.47	Joback Method
cpg	1623.76	J/molxK	1090.03	Joback Method
dvisc	0.0000222	Paxs	885.36	Joback Method

dvisc	0.0000315	Paxs	806.61	Joback Method
dvisc	0.0000482	Paxs	727.86	Joback Method
dvisc	0.0000818	Paxs	649.11	Joback Method
dvisc	0.0001607	Paxs	570.36	Joback Method
dvisc	0.0003919	Paxs	491.61	Joback Method
dvisc	0.0013422	Paxs	412.86	Joback Method

## Sources

<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=R300717&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R300717&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>

## Legend

<b>cp<sub>g</sub>:</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>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</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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