

# 2-Heneicosene (E)

Inchi:	InChI=1S/C21H42/c1-3-5-7-9-11-13-15-17-19-21-20-18-16-14-12-10-8-6-4-2/h3,5H,4,6-2
InchiKey:	SEPFQHJECFKHGD-HWKANZROSA-N
Formula:	C21H42
SMILES:	CC=CCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	294.56

## Physical Properties

Property code	Value	Unit	Source
gf	206.16	kJ/mol	Joback Method
hf	-359.55	kJ/mol	Joback Method
hfus	50.35	kJ/mol	Joback Method
hvap	62.30	kJ/mol	Joback Method
log10ws	-8.47		Crippen Method
logp	8.214		Crippen Method
mcvol	302.450	ml/mol	McGowan Method
pc	987.64	kPa	Joback Method
rinsol	2107.00		NIST Webbook
tb	684.04	K	Joback Method
tc	849.41	K	Joback Method
tf	321.35	K	Joback Method
vc	1.192	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.54	J/molxK	684.04	Joback Method
cpg	975.47	J/molxK	821.85	Joback Method
cpg	957.94	J/molxK	794.28	Joback Method
cpg	939.61	J/molxK	766.72	Joback Method
cpg	920.46	J/molxK	739.16	Joback Method
cpg	900.45	J/molxK	711.60	Joback Method
cpg	992.25	J/molxK	849.41	Joback Method
dvisc	0.0000740	Paxs	684.04	Joback Method
dvisc	0.0001020	Paxs	623.59	Joback Method

dvisc	0.0001506	Paxs	563.14	Joback Method
dvisc	0.0002442	Paxs	502.69	Joback Method
dvisc	0.0004519	Paxs	442.25	Joback Method
dvisc	0.0010163	Paxs	381.80	Joback Method
dvisc	0.0031008	Paxs	321.35	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=R205706&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R205706&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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