

# 3,3-Diethylheptadecane

<b>Inchi:</b>	InChI=1S/C21H44/c1-5-9-10-11-12-13-14-15-16-17-18-19-20-21(6-2,7-3)8-4/h5-20H2,1-
<b>InchiKey:</b>	ZEFHGRZKMZQAKZ-UHFFFAOYSA-N
<b>Formula:</b>	C21H44
<b>SMILES:</b>	CCCCCCCCCCCCCCC(CC)(CC)CC
<b>Mol. weight [g/mol]:</b>	296.57

## Physical Properties

Property code	Value	Unit	Source
gf	128.78	kJ/mol	Joback Method
hf	-485.52	kJ/mol	Joback Method
hfus	42.73	kJ/mol	Joback Method
hvap	61.04	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	8.294		Crippen Method
mcvol	306.750	ml/mol	McGowan Method
pc	967.47	kPa	Joback Method
rinsol	2061.00		NIST Webbook
tb	676.65	K	Joback Method
tc	842.53	K	Joback Method
tf	328.85	K	Joback Method
vc	1.200	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	902.40	J/molxK	676.65	Joback Method
cpg	1001.89	J/molxK	814.88	Joback Method
cpg	983.77	J/molxK	787.24	Joback Method
cpg	964.81	J/molxK	759.59	Joback Method
cpg	944.95	J/molxK	731.94	Joback Method
cpg	924.16	J/molxK	704.30	Joback Method
cpg	1019.20	J/molxK	842.53	Joback Method
dvisc	0.0000729	Paxs	676.65	Joback Method
dvisc	0.0001035	Paxs	618.68	Joback Method

dvisc	0.0001579	Paxs	560.72	Joback Method
dvisc	0.0002656	Paxs	502.75	Joback Method
dvisc	0.0005115	Paxs	444.78	Joback Method
dvisc	0.0011988	Paxs	386.82	Joback Method
dvisc	0.0037943	Paxs	328.85	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U360416&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360416&amp;Units=SI</a>
<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>

## 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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