

# Octadecane, 3-methyl-

<b>Other names:</b>	3-Methyloctadecane
<b>Inchi:</b>	InChI=1S/C19H40/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19(3)5-2/h19H,4-18H2,1-3H
<b>InchiKey:</b>	PGZRTPKNSFMAOP-UHFFFAOYSA-N
<b>Formula:</b>	C19H40
<b>SMILES:</b>	CCCCCCCCCCCCCCCC(C)CC
<b>Mol. weight [g/mol]:</b>	268.52
<b>CAS:</b>	6561-44-0

## Physical Properties

Property code	Value	Unit	Source
gf	106.66	kJ/mol	Joback Method
hf	-440.77	kJ/mol	Joback Method
hfus	41.44	kJ/mol	Joback Method
hvap	57.50	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	7.514		Crippen Method
mcvol	278.570	ml/mol	McGowan Method
pc	1086.35	kPa	Joback Method
tb	633.68	K	Joback Method
tc	794.96	K	Joback Method
tf	288.89	K	Joback Method
vc	1.093	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.70	J/molxK	633.68	Joback Method
cpg	802.48	J/molxK	660.56	Joback Method
cpg	822.41	J/molxK	687.44	Joback Method
cpg	841.51	J/molxK	714.32	Joback Method
cpg	859.82	J/molxK	741.20	Joback Method
cpg	877.35	J/molxK	768.08	Joback Method
cpg	894.13	J/molxK	794.96	Joback Method
dvisc	0.0057089	Paxs	288.89	Joback Method

dvisc	0.0016729	Paxs	346.36	Joback Method
dvisc	0.0006952	Paxs	403.82	Joback Method
dvisc	0.0003595	Paxs	461.29	Joback Method
dvisc	0.0002152	Paxs	518.75	Joback Method
dvisc	0.0001427	Paxs	576.22	Joback Method
dvisc	0.0001019	Paxs	633.68	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42061e+01
Coeff. B	-4.45449e+03
Coeff. C	-1.35550e+02
Temperature range (K), min.	455.59
Temperature range (K), max.	636.36

## Sources

**The Yaws Handbook of Vapor**

**Pressure:  
Crippen Method:**

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci990307i>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C6561440&Units=SI>

## 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>pvap:</b>	Vapor pressure
<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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