

# Pentadecane, 3-methyl-

<b>Other names:</b>	3-Methylpentadecane
<b>Inchi:</b>	InChI=1S/C16H34/c1-4-6-7-8-9-10-11-12-13-14-15-16(3)5-2/h16H,4-15H2,1-3H3
<b>InchiKey:</b>	FWXKCXJPHSAYMK-UHFFFAOYSA-N
<b>Formula:</b>	C16H34
<b>SMILES:</b>	CCCCCCCCCCCC(C)CC
<b>Mol. weight [g/mol]:</b>	226.44
<b>CAS:</b>	2882-96-4

## Physical Properties

Property code	Value	Unit	Source
gf	81.40	kJ/mol	Joback Method
hf	-378.85	kJ/mol	Joback Method
hfus	33.67	kJ/mol	Joback Method
hvap	50.82	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	6.344		Crippen Method
mcvol	236.300	ml/mol	McGowan Method
pc	1326.17	kPa	Joback Method
rinpol	1570.93		NIST Webbook
rinpol	1571.48		NIST Webbook
rinpol	1571.51		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1571.00		NIST Webbook
rinpol	1572.70		NIST Webbook
rinpol	1566.00		NIST Webbook
rinpol	1572.06		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1569.00		NIST Webbook
rinpol	1571.82		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1568.60		NIST Webbook
rinpol	1572.06		NIST Webbook
rinpol	1571.46		NIST Webbook
rinpol	1572.00		NIST Webbook
rinpol	1570.20		NIST Webbook

rinpol	1568.60		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1572.00		NIST Webbook
rinpol	1569.00		NIST Webbook
tb	539.50 ± 3.00	K	NIST Webbook
tc	726.28	K	Joback Method
tf	250.90 ± 0.60	K	NIST Webbook
tf	241.20 ± 1.00	K	NIST Webbook
tf	250.20 ± 2.00	K	NIST Webbook
vc	0.925	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.96	J/molxK	565.04	Joback Method
cpg	631.47	J/molxK	591.91	Joback Method
cpg	650.21	J/molxK	618.79	Joback Method
cpg	668.20	J/molxK	645.66	Joback Method
cpg	685.47	J/molxK	672.53	Joback Method
cpg	702.03	J/molxK	699.40	Joback Method
cpg	717.90	J/molxK	726.28	Joback Method
dvisc	0.0077044	Paxs	255.08	Joback Method
dvisc	0.0022640	Paxs	306.74	Joback Method
dvisc	0.0009470	Paxs	358.40	Joback Method
dvisc	0.0004934	Paxs	410.06	Joback Method
dvisc	0.0002974	Paxs	461.72	Joback Method
dvisc	0.0001985	Paxs	513.38	Joback Method
dvisc	0.0001427	Paxs	565.04	Joback Method
hvapt	61.00	kJ/mol	486.00	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42755e+01
Coeff. B	-4.21487e+03

Coeff. C	-1.18700e+02
Temperature range (K), min.	420.02
Temperature range (K), max.	588.90

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2882964&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2882964&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</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>h vap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>r inpol:</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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