

# Undecane, 3-methyl-

<b>Other names:</b>	(dl) 3-methylundecane 2-Ethyl-decane 3-Methylundecane
<b>Inchi:</b>	InChI=1S/C12H26/c1-4-6-7-8-9-10-11-12(3)5-2/h12H,4-11H2,1-3H3
<b>InchiKey:</b>	HTZWVZNRDDOFEI-UHFFFAOYSA-N
<b>Formula:</b>	C12H26
<b>SMILES:</b>	CCCCCCCC(C)CC
<b>Mol. weight [g/mol]:</b>	170.33
<b>CAS:</b>	1002-43-3

## Physical Properties

Property code	Value	Unit	Source
gf	47.72	kJ/mol	Joback Method
hf	-296.29	kJ/mol	Joback Method
hfus	23.31	kJ/mol	Joback Method
hvap	41.92	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.783		Crippen Method
mcvol	179.940	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
rinpol	1168.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1169.60		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1173.00		NIST Webbook

rinpol	1172.20		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1170.00		NIST Webbook
tb	473.52	K	Joback Method
tc	637.74	K	Joback Method
tf	218.50 ± 2.00	K	NIST Webbook
tf	215.20 ± 5.00	K	NIST Webbook
vc	0.702	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.90	J/molxK	473.52	Joback Method
cpg	424.06	J/molxK	500.89	Joback Method
cpg	440.58	J/molxK	528.26	Joback Method
cpg	456.45	J/molxK	555.63	Joback Method
cpg	471.71	J/molxK	583.00	Joback Method
cpg	486.36	J/molxK	610.37	Joback Method
cpg	500.43	J/molxK	637.74	Joback Method
dvisc	0.0101808	Paxs	210.00	Joback Method
dvisc	0.0030132	Paxs	253.92	Joback Method
dvisc	0.0012770	Paxs	297.84	Joback Method
dvisc	0.0006749	Paxs	341.76	Joback Method
dvisc	0.0004124	Paxs	385.68	Joback Method
dvisc	0.0002787	Paxs	429.60	Joback Method
dvisc	0.0002026	Paxs	473.52	Joback Method
hvapt	48.80	kJ/mol	421.00	NIST Webbook

rho1	758.60	kg/m3	283.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rho1	751.30	kg/m3	293.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rho1	744.00	kg/m3	303.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rho1	736.70	kg/m3	313.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rho1	729.30	kg/m3	323.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rho1	721.90	kg/m3	333.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rho1	714.40	kg/m3	343.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels

rho1	707.00	kg/m3	353.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rho1	699.40	kg/m3	363.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rho1	691.90	kg/m3	373.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rho1	758.30	kg/m3	283.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rho1	751.10	kg/m3	293.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rho1	743.90	kg/m3	303.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rho1	736.60	kg/m3	313.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels

rhoI	729.30	kg/m <sup>3</sup>	323.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
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## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41901e+01
Coeff. B	-3.75824e+03
Coeff. C	-9.13150e+01
Temperature range (K), min.	361.64
Temperature range (K), max.	514.60

## Sources

<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=C1002433&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1002433&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>Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels:</b>	<a href="https://www.doi.org/10.1021/je400274f">https://www.doi.org/10.1021/je400274f</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>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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rho:</b>	Liquid Density
<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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