

# Undecane, 5-methyl-

<b>Other names:</b>	5-Methylundecane Methylundecane
<b>Inchi:</b>	InChI=1S/C12H26/c1-4-6-8-9-11-12(3)10-7-5-2/h12H,4-11H2,1-3H3
<b>InchiKey:</b>	QULNVKABFWNUCW-UHFFFAOYSA-N
<b>Formula:</b>	C12H26
<b>SMILES:</b>	CCCCCCC(C)CCCC
<b>Mol. weight [g/mol]:</b>	170.33
<b>CAS:</b>	1632-70-8

## 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	1158.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1153.60		NIST Webbook
rinpol	1154.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1157.14		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1157.24		NIST Webbook
rinpol	1156.30		NIST Webbook
rinpol	1153.60		NIST Webbook
rinpol	1156.52		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1154.00		NIST Webbook
rinpol	1156.00		NIST Webbook

rinpol	1157.40		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1193.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1157.29		NIST Webbook
rinpol	1156.62		NIST Webbook
rinpol	1152.00		NIST Webbook
ripol	1157.00		NIST Webbook
tb	473.52	K	Joback Method
tc	637.74	K	Joback Method
tf	205.40 ± 2.00	K	NIST Webbook
vc	0.702	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.43	J/molxK	637.74	Joback Method
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
dvisc	0.0002026	Paxs	473.52	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
hvapt	50.30	kJ/mol	418.50	NIST Webbook

# Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41966e+01
Coeff. B	-3.71480e+03
Coeff. C	-9.13150e+01
Temperature range (K), min.	358.39
Temperature range (K), max.	509.41

## Sources

<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=C1632708&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1632708&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>

## 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>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices

**tb:** Normal Boiling Point Temperature  
**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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