

# Undecane, 2,2-dimethyl-

<b>Other names:</b>	2,2-Dimethylundecane
<b>Inchi:</b>	InChI=1S/C13H28/c1-5-6-7-8-9-10-11-12-13(2,3)4/h5-12H2,1-4H3
<b>InchiKey:</b>	QDKSGHXRHXVMPF-UHFFFAOYSA-N
<b>Formula:</b>	C13H28
<b>SMILES:</b>	CCCCCCCCC(C)(C)C
<b>Mol. weight [g/mol]:</b>	184.36
<b>CAS:</b>	17312-64-0

## Physical Properties

Property code	Value	Unit	Source
gf	61.42	kJ/mol	Joback Method
hf	-320.40	kJ/mol	Joback Method
hfus	22.01	kJ/mol	Joback Method
hvap	43.24	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	5.173		Crippen Method
mcvol	194.030	ml/mol	McGowan Method
pc	1670.06	kPa	Joback Method
rinpol	1214.00		NIST Webbook
rinpol	1218.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1215.00		NIST Webbook
tb	493.61	K	Joback Method
tc	662.67	K	Joback Method
tf	238.69	K	Joback Method
vc	0.752	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.75	J/molxK	493.61	Joback Method
cpg	476.43	J/molxK	521.79	Joback Method
cpg	494.29	J/molxK	549.96	Joback Method
cpg	511.35	J/molxK	578.14	Joback Method

cpg	527.65	J/mol×K	606.32	Joback Method
cpg	543.21	J/mol×K	634.50	Joback Method
cpg	558.07	J/mol×K	662.67	Joback Method
dvisc	0.0090102	Paxs	238.69	Joback Method
dvisc	0.0029290	Paxs	281.18	Joback Method
dvisc	0.0012789	Paxs	323.66	Joback Method
dvisc	0.0006768	Paxs	366.15	Joback Method
dvisc	0.0004088	Paxs	408.64	Joback Method
dvisc	0.0002716	Paxs	451.12	Joback Method
dvisc	0.0001935	Paxs	493.61	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.39643e+01
Coeff. B	-3.69372e+03
Coeff. C	-9.89300e+01
Temperature range (K), min.	369.00
Temperature range (K), max.	525.81

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C17312640&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C17312640&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>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>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

Latest version available from:

<https://www.cheméo.com/cid/60-889-9/Undecane-2-2-dimethyl.pdf>

Generated by Cheméo on 2024-04-17 16:54:14.789395959 +0000 UTC m=+15662103.709973274.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.