

# 3-Methylundecanol

<b>Inchi:</b>	InChI=1S/C12H26O/c1-3-4-5-6-7-8-9-12(2)10-11-13/h12-13H,3-11H2,1-2H3
<b>InchiKey:</b>	CTVPPKBJEDDIHQ-UHFFFAOYSA-N
<b>Formula:</b>	C12H26O
<b>SMILES:</b>	CCCCCCCC(C)CCO
<b>Mol. weight [g/mol]:</b>	186.33
<b>CAS:</b>	---

## Physical Properties

Property code	Value	Unit	Source
gf	-89.10	kJ/mol	Joback Method
hf	-448.52	kJ/mol	Joback Method
hfus	27.40	kJ/mol	Joback Method
hvap	58.60	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.756		Crippen Method
mcvol	185.810	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	1336.00		NIST Webbook
tb	565.70	K	Joback Method
tc	725.92	K	Joback Method
tf	270.82	K	Joback Method
vc	0.721	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.70	J/molxK	565.70	Joback Method
cpg	493.60	J/molxK	592.40	Joback Method
cpg	507.92	J/molxK	619.11	Joback Method
cpg	521.66	J/molxK	645.81	Joback Method
cpg	534.85	J/molxK	672.51	Joback Method
cpg	547.50	J/molxK	699.22	Joback Method
cpg	559.62	J/molxK	725.92	Joback Method
dvisc	0.0381702	Paxs	270.82	Joback Method

dvisc	0.0062239	Paxs	319.97	Joback Method
dvisc	0.0016449	Paxs	369.11	Joback Method
dvisc	0.0005944	Paxs	418.26	Joback Method
dvisc	0.0002660	Paxs	467.41	Joback Method
dvisc	0.0001387	Paxs	516.55	Joback Method
dvisc	0.0000810	Paxs	565.70	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.58487e+01
Coeff. B	-4.92640e+03
Coeff. C	-8.53350e+01
Temperature range (K), min.	401.92
Temperature range (K), max.	552.86

## Sources

NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R407937&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R407937&amp;Units=SI</a>
The Yaws Handbook of Vapor Pressure:	<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>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
Joback Method:	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
McGowan Method:	<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>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>rinpola:</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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