

# Undecane, 5-ethyl-

<b>Inchi:</b>	InChI=1S/C13H28/c1-4-7-9-10-12-13(6-3)11-8-5-2/h13H,4-12H2,1-3H3
<b>InchiKey:</b>	MKHPXJRMKJYYON-UHFFFAOYSA-N
<b>Formula:</b>	C13H28
<b>SMILES:</b>	CCCCCCC(CC)CCCC
<b>Mol. weight [g/mol]:</b>	184.36
<b>CAS:</b>	17453-94-0

## Physical Properties

Property code	Value	Unit	Source
gf	56.14	kJ/mol	Joback Method
hf	-316.93	kJ/mol	Joback Method
hfus	25.90	kJ/mol	Joback Method
hvap	44.14	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	5.173		Crippen Method
mcvol	194.030	ml/mol	McGowan Method
pc	1655.15	kPa	Joback Method
rinpol	1232.00		NIST Webbook
tb	496.40	K	Joback Method
tc	659.72	K	Joback Method
tf	221.27	K	Joback Method
vc	0.757	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.59	J/molxK	496.40	Joback Method
cpg	473.45	J/molxK	523.62	Joback Method
cpg	490.62	J/molxK	550.84	Joback Method
cpg	507.13	J/molxK	578.06	Joback Method
cpg	522.98	J/molxK	605.28	Joback Method
cpg	538.20	J/molxK	632.50	Joback Method
cpg	552.81	J/molxK	659.72	Joback Method
dvisc	0.0096568	Paxs	221.27	Joback Method

dvisc	0.0028515	Paxs	267.12	Joback Method
dvisc	0.0012038	Paxs	312.98	Joback Method
dvisc	0.0006335	Paxs	358.83	Joback Method
dvisc	0.0003856	Paxs	404.69	Joback Method
dvisc	0.0002596	Paxs	450.54	Joback Method
dvisc	0.0001881	Paxs	496.40	Joback Method

## 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=C17453940&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C17453940&amp;Units=SI</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>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>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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