

# Octane, 4-ethyl-3-methyl

<b>Inchi:</b>	InChI=1S/C11H24/c1-5-8-9-11(7-3)10(4)6-2/h10-11H,5-9H2,1-4H3
<b>InchiKey:</b>	BTRAURWAFYPYMW-UHFFFAOYSA-N
<b>Formula:</b>	C11H24
<b>SMILES:</b>	CCCCC(CC)C(C)CC
<b>Mol. weight [g/mol]:</b>	156.31

## Physical Properties

Property code	Value	Unit	Source
gf	36.86	kJ/mol	Joback Method
hf	-280.93	kJ/mol	Joback Method
hfus	17.20	kJ/mol	Joback Method
hvap	39.30	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	4.249		Crippen Method
mcvol	165.850	ml/mol	McGowan Method
pc	1961.34	kPa	Joback Method
rinpola	1017.00		NIST Webbook
tb	450.20	K	Joback Method
tc	618.81	K	Joback Method
tf	183.73	K	Joback Method
vc	0.639	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.12	J/molxK	450.20	Joback Method
cpg	437.81	J/molxK	590.71	Joback Method
cpg	423.51	J/molxK	562.61	Joback Method
cpg	408.60	J/molxK	534.51	Joback Method
cpg	393.08	J/molxK	506.40	Joback Method
cpg	376.92	J/molxK	478.30	Joback Method
cpg	451.53	J/molxK	618.81	Joback Method
dvisc	0.0002057	Paxs	450.20	Joback Method
dvisc	0.0002907	Paxs	405.79	Joback Method

dvisc	0.0004471	Paxs	361.38	Joback Method
dvisc	0.0007760	Paxs	316.96	Joback Method
dvisc	0.0016118	Paxs	272.55	Joback Method
dvisc	0.0044499	Paxs	228.14	Joback Method
dvisc	0.0200727	Paxs	183.73	Joback Method

## 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=R9539&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R9539&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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