

# Heptane, 3-ethyl-2-methyl-

<b>Other names:</b>	2-METHYL-3-ETHYLHEPTANE 3-ETHYL-2-METHYLHEPTANE
<b>Inchi:</b>	InChI=1S/C10H22/c1-5-7-8-10(6-2)9(3)4/h9-10H,5-8H2,1-4H3
<b>InchiKey:</b>	NKMJCVVUYDKHAV-UHFFFAOYSA-N
<b>Formula:</b>	C10H22
<b>SMILES:</b>	CCCCC(CC)C(C)C
<b>Mol. weight [g/mol]:</b>	142.28
<b>CAS:</b>	14676-29-0

## Physical Properties

Property code	Value	Unit	Source
gf	28.44	kJ/mol	Joback Method
hf	-260.29	kJ/mol	Joback Method
hfus	14.61	kJ/mol	Joback Method
hvap	48.10	kJ/mol	NIST Webbook
log10ws	-3.52		Crippen Method
logp	3.859		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2139.38	kPa	Joback Method
rinpol	946.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	941.70		NIST Webbook
rinpol	941.80		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	942.40		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	938.00		NIST Webbook
rinpol	942.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	940.65		NIST Webbook
tb	427.32	K	Joback Method
tc	596.92	K	Joback Method

tf	172.46	K	Joback Method
vc	0.584	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.26	J/mol×K	427.32	Joback Method
cpg	388.93	J/mol×K	568.65	Joback Method
cpg	375.35	J/mol×K	540.39	Joback Method
cpg	361.21	J/mol×K	512.12	Joback Method
cpg	346.50	J/mol×K	483.85	Joback Method
cpg	331.18	J/mol×K	455.59	Joback Method
cpg	401.95	J/mol×K	596.92	Joback Method
dvisc	0.0002171	Paxs	427.32	Joback Method
dvisc	0.0003059	Paxs	384.84	Joback Method
dvisc	0.0004693	Paxs	342.37	Joback Method
dvisc	0.0008129	Paxs	299.89	Joback Method
dvisc	0.0016877	Paxs	257.41	Joback Method
dvisc	0.0046771	Paxs	214.94	Joback Method
dvisc	0.0214146	Paxs	172.46	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42650e+01
Coeff. B	-3.61192e+03
Coeff. C	-5.99360e+01
Temperature range (K), min.	318.35
Temperature range (K), max.	463.35

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.02506e+02
Coeff. B	-9.13884e+03

Coeff. C	-1.28894e+01
Coeff. D	7.63903e-06
Temperature range (K), min.	318.15
Temperature range (K), max.	610.90

## Sources

<b>KDB Vapor Pressure Data:</b>	<a href="https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=118">https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=118</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemed.com/doc/models/crippen_log10ws">https://www.chemed.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>KDB:</b>	<a href="https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=118">https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=118</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=C14676290&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C14676290&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>

## 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>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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