

# Heptane, 2,2,3-trimethyl-

<b>Other names:</b>	2,2,3-Trimethylheptane
<b>Inchi:</b>	InChI=1S/C10H22/c1-6-7-8-9(2)10(3,4)5/h9H,6-8H2,1-5H3
<b>InchiKey:</b>	ACYHSTUWOQNWGX-UHFFFAOYSA-N
<b>Formula:</b>	C10H22
<b>SMILES:</b>	CCCCC(C)C(C)(C)C
<b>Mol. weight [g/mol]:</b>	142.28
<b>CAS:</b>	52896-92-1

## Physical Properties

Property code	Value	Unit	Source
gf	33.72	kJ/mol	Joback Method
hf	-263.76	kJ/mol	Joback Method
hfus	10.72	kJ/mol	Joback Method
hvap	46.90	kJ/mol	NIST Webbook
log10ws	-3.52		Crippen Method
logp	3.859		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
rinpol	922.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	914.40		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	912.70		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	914.00		NIST Webbook
tb	424.53	K	Joback Method
tc	600.93	K	Joback Method
tf	189.88	K	Joback Method
vc	0.579	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.93	J/molxK	424.53	Joback Method
cpg	333.94	J/molxK	453.93	Joback Method
cpg	350.18	J/molxK	483.33	Joback Method
cpg	365.66	J/molxK	512.73	Joback Method
cpg	380.41	J/molxK	542.13	Joback Method
cpg	394.47	J/molxK	571.53	Joback Method
cpg	407.85	J/molxK	600.93	Joback Method
dvisc	0.0206027	Paxs	189.88	Joback Method
dvisc	0.0052013	Paxs	228.99	Joback Method
dvisc	0.0019620	Paxs	268.10	Joback Method
dvisc	0.0009486	Paxs	307.20	Joback Method
dvisc	0.0005405	Paxs	346.31	Joback Method
dvisc	0.0003452	Paxs	385.42	Joback Method
dvisc	0.0002394	Paxs	424.53	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.40606e+01
Coeff. B	-3.47994e+03
Coeff. C	-6.22090e+01
Temperature range (K), min.	314.87
Temperature range (K), max.	459.96

## 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=C52896921&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C52896921&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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