

# Benzene, 1-heptyl-4-methyl

Inchi:	InChI=1S/C14H22/c1-3-4-5-6-7-8-14-11-9-13(2)10-12-14/h9-12H,3-8H2,1-2H3
InchiKey:	RYEBGSXADPCJTG-UHFFFAOYSA-N
Formula:	C14H22
SMILES:	CCCCCCCc1ccc(C)cc1
Mol. weight [g/mol]:	190.32

## Physical Properties

Property code	Value	Unit	Source
gf	169.78	kJ/mol	Joback Method
hf	-107.23	kJ/mol	Joback Method
hfus	25.67	kJ/mol	Joback Method
hvap	49.70	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.508		Crippen Method
mcvol	184.360	ml/mol	McGowan Method
pc	1982.35	kPa	Joback Method
ripol	1434.00		NIST Webbook
ripol	1742.00		NIST Webbook
ripol	1729.00		NIST Webbook
ripol	1713.00		NIST Webbook
ripol	1697.60		NIST Webbook
ripol	1691.00		NIST Webbook
ripol	1691.00		NIST Webbook
ripol	1691.00		NIST Webbook
ripol	1697.60		NIST Webbook
ripol	1699.00		NIST Webbook
tb	551.38	K	Joback Method
tc	746.43	K	Joback Method
tf	286.48	K	Joback Method
vc	0.712	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	442.44	J/molxK	551.38	Joback Method
cpg	460.30	J/molxK	583.89	Joback Method
cpg	477.25	J/molxK	616.40	Joback Method
cpg	493.33	J/molxK	648.91	Joback Method
cpg	508.57	J/molxK	681.42	Joback Method
cpg	522.99	J/molxK	713.92	Joback Method
cpg	536.64	J/molxK	746.43	Joback Method
dvisc	0.0026153	Paxs	286.48	Joback Method
dvisc	0.0012344	Paxs	330.63	Joback Method
dvisc	0.0006953	Paxs	374.78	Joback Method
dvisc	0.0004420	Paxs	418.93	Joback Method
dvisc	0.0003064	Paxs	463.08	Joback Method
dvisc	0.0002263	Paxs	507.23	Joback Method
dvisc	0.0001755	Paxs	551.38	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R12618&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R12618&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<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>

## 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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature

**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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