

# Benzene, (1-methylenebutyl)-

<b>Other names:</b>	2-Phenyl-1-pentene
<b>Inchi:</b>	InChI=1S/C11H14/c1-3-7-10(2)11-8-5-4-6-9-11/h4-6,8-9H,2-3,7H2,1H3
<b>InchiKey:</b>	ANGVCCXFJKHNDS-UHFFFAOYSA-N
<b>Formula:</b>	C11H14
<b>SMILES:</b>	C=C(CCC)c1ccccc1
<b>Mol. weight [g/mol]:</b>	146.23
<b>CAS:</b>	5676-32-4

## Physical Properties

Property code	Value	Unit	Source
gf	233.44	kJ/mol	Joback Method
hf	81.80	kJ/mol	Joback Method
hfus	15.70	kJ/mol	Joback Method
hvap	41.77	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.500		Crippen Method
mcvol	137.790	ml/mol	McGowan Method
pc	2781.78	kPa	Joback Method
rinpol	1236.30		NIST Webbook
rinpol	1236.30		NIST Webbook
tb	474.15 ± 2.00	K	NIST Webbook
tc	684.75	K	Joback Method
tf	224.43	K	Joback Method
vc	0.525	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.40	J/mol×K	474.32	Joback Method
cpg	298.13	J/mol×K	509.39	Joback Method
cpg	312.92	J/mol×K	544.46	Joback Method
cpg	326.83	J/mol×K	579.53	Joback Method
cpg	339.88	J/mol×K	614.61	Joback Method
cpg	352.13	J/mol×K	649.68	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5676324&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5676324&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>
<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>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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