

# Benzene, (2-methyl-1-methylenepropyl)-

<b>Other names:</b>	«alpha»-isopropylstyrene
<b>Inchi:</b>	InChI=1S/C11H14/c1-9(2)10(3)11-7-5-4-6-8-11/h4-9H,3H2,1-2H3
<b>InchiKey:</b>	POZGETMIPGBFGQ-UHFFFAOYSA-N
<b>Formula:</b>	C11H14
<b>SMILES:</b>	<chem>C=C(c1ccccc1)C(C)C</chem>
<b>Mol. weight [g/mol]:</b>	146.23
<b>CAS:</b>	17498-71-4

## Physical Properties

Property code	Value	Unit	Source
gf	231.00	kJ/mol	Joback Method
hf	76.52	kJ/mol	Joback Method
hfus	12.17	kJ/mol	Joback Method
hvap	53.30 ± 0.30	kJ/mol	NIST Webbook
log10ws	-3.31		Crippen Method
logp	3.356		Crippen Method
mcvol	137.790	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
tb	465.15 ± 2.00	K	NIST Webbook
tc	689.29	K	Joback Method
tf	209.43	K	Joback Method
vc	0.519	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.55	J/mol×K	473.88	Joback Method
cpg	298.74	J/mol×K	509.78	Joback Method
cpg	313.94	J/mol×K	545.68	Joback Method
cpg	328.19	J/mol×K	581.58	Joback Method
cpg	341.55	J/mol×K	617.48	Joback Method
cpg	354.06	J/mol×K	653.38	Joback Method
cpg	365.76	J/mol×K	689.29	Joback Method

# Sources

<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=C17498714&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C17498714&amp;Units=SI</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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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>hvac:</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>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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