

# Benzene, (1,3-dimethyl-2-butenyl)-

<b>Inchi:</b>	InChI=1S/C12H16/c1-10(2)9-11(3)12-7-5-4-6-8-12/h4-9,11H,1-3H3
<b>InchiKey:</b>	NKDQCWOVRPPHEF-UHFFFAOYSA-N
<b>Formula:</b>	C12H16
<b>SMILES:</b>	CC(C)=CC(C)c1ccccc1
<b>Mol. weight [g/mol]:</b>	160.26
<b>CAS:</b>	50704-01-3

## Physical Properties

Property code	Value	Unit	Source
gf	231.80	kJ/mol	Joback Method
hf	47.67	kJ/mol	Joback Method
hfus	16.25	kJ/mol	Joback Method
hvap	44.23	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.756		Crippen Method
mcvol	151.880	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
tb	504.24	K	Joback Method
tc	721.85	K	Joback Method
tf	217.38	K	Joback Method
vc	0.575	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.34	J/molxK	504.24	Joback Method
cpg	345.62	J/molxK	540.51	Joback Method
cpg	361.80	J/molxK	576.78	Joback Method
cpg	376.94	J/molxK	613.04	Joback Method
cpg	391.11	J/molxK	649.31	Joback Method
cpg	404.36	J/molxK	685.58	Joback Method
cpg	416.75	J/molxK	721.85	Joback Method

# 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=C50704013&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C50704013&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>

# 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>mccol:</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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