

# 2-Methyl-1-phenyl-1-butanol

<b>Inchi:</b>	InChI=1S/C11H16O/c1-3-9(2)11(12)10-7-5-4-6-8-10/h4-9,11-12H,3H2,1-2H3
<b>InchiKey:</b>	XYQQWQIEEXLXDX-UHFFFAOYSA-N
<b>Formula:</b>	C11H16O
<b>SMILES:</b>	CCC(C)C(O)c1ccccc1
<b>Mol. weight [g/mol]:</b>	164.24
<b>CAS:</b>	3968-86-3

## Physical Properties

Property code	Value	Unit	Source
gf	12.45	kJ/mol	Joback Method
hf	-196.63	kJ/mol	Joback Method
hfus	15.33	kJ/mol	Joback Method
hvap	58.26	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.766		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
tb	569.06	K	Joback Method
tc	766.75	K	Joback Method
tf	270.97	K	Joback Method
vc	0.550	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.21	J/molxK	569.06	Joback Method
cpg	421.10	J/molxK	733.80	Joback Method
cpg	410.17	J/molxK	700.86	Joback Method
cpg	398.55	J/molxK	667.91	Joback Method
cpg	386.21	J/molxK	634.96	Joback Method
cpg	373.11	J/molxK	602.01	Joback Method
cpg	431.36	J/molxK	766.75	Joback Method
dvisc	0.0000795	Paxs	569.06	Joback Method
dvisc	0.0001356	Paxs	519.38	Joback Method

dvisc	0.0002589	Paxs	469.70	Joback Method
dvisc	0.0005758	Paxs	420.01	Joback Method
dvisc	0.0015874	Paxs	370.33	Joback Method
dvisc	0.0059917	Paxs	320.65	Joback Method
dvisc	0.0368090	Paxs	270.97	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3968863&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3968863&amp;Units=SI</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>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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