

# (2-Methylphenyl) methanol, n-butyl ether

Inchi:	InChI=1S/C12H18O/c1-3-4-9-13-10-12-8-6-5-7-11(12)2/h5-8H,3-4,9-10H2,1-2H3
InchiKey:	VGGGYTKIMSSOER-UHFFFAOYSA-N
Formula:	C12H18O
SMILES:	CCCCOCc1ccccc1C
Mol. weight [g/mol]:	178.27

## Physical Properties

Property code	Value	Unit	Source
gf	47.94	kJ/mol	Joback Method
hf	-198.17	kJ/mol	Joback Method
hfus	21.68	kJ/mol	Joback Method
hvap	47.65	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.312		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
rinpol	1361.00		NIST Webbook
tb	528.04	K	Joback Method
tc	726.82	K	Joback Method
tf	286.17	K	Joback Method
vc	0.618	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.37	J/mol×K	528.04	Joback Method
cpg	388.47	J/mol×K	561.17	Joback Method
cpg	403.80	J/mol×K	594.30	Joback Method
cpg	418.37	J/mol×K	627.43	Joback Method
cpg	432.20	J/mol×K	660.56	Joback Method
cpg	445.32	J/mol×K	693.69	Joback Method
cpg	457.72	J/mol×K	726.82	Joback Method
dvisc	0.0019790	Paxs	286.17	Joback Method
dvisc	0.0010163	Paxs	326.48	Joback Method

dvisc	0.0006042	Paxs	366.79	Joback Method
dvisc	0.0003982	Paxs	407.11	Joback Method
dvisc	0.0002829	Paxs	447.42	Joback Method
dvisc	0.0002127	Paxs	487.73	Joback Method
dvisc	0.0001670	Paxs	528.04	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=U374706&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U374706&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>

## 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>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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