

# (3-Methylphenyl) methanol, 2-methylpropyl ether

Inchi:	InChI=1S/C12H18O/c1-10(2)8-13-9-12-6-4-5-11(3)7-12/h4-7,10H,8-9H2,1-3H3
InchiKey:	IYDGSOYVMNWCIR-UHFFFAOYSA-N
Formula:	C12H18O
SMILES:	Cc1cccc(COCC(C)C)c1
Mol. weight [g/mol]:	178.27

## Physical Properties

Property code	Value	Unit	Source
gf	45.50	kJ/mol	Joback Method
hf	-203.45	kJ/mol	Joback Method
hfus	18.15	kJ/mol	Joback Method
hvap	47.27	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	3.168		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
rinpol	1302.00		NIST Webbook
tb	527.60	K	Joback Method
tc	730.68	K	Joback Method
tf	271.17	K	Joback Method
vc	0.612	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.63	J/mol×K	527.60	Joback Method
cpg	389.15	J/mol×K	561.45	Joback Method
cpg	404.85	J/mol×K	595.29	Joback Method
cpg	419.75	J/mol×K	629.14	Joback Method
cpg	433.88	J/mol×K	662.99	Joback Method
cpg	447.24	J/mol×K	696.83	Joback Method
cpg	459.86	J/mol×K	730.68	Joback Method
dvisc	0.0026822	Paxs	271.17	Joback Method
dvisc	0.0012118	Paxs	313.91	Joback Method

dvisc	0.0006624	Paxs	356.65	Joback Method
dvisc	0.0004120	Paxs	399.38	Joback Method
dvisc	0.0002809	Paxs	442.12	Joback Method
dvisc	0.0002049	Paxs	484.86	Joback Method
dvisc	0.0001573	Paxs	527.60	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U374582&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U374582&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>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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