

# (3-Methylphenyl) methanol, 3-methylbutyl ether

Inchi:	InChI=1S/C13H20O/c1-11(2)7-8-14-10-13-6-4-5-12(3)9-13/h4-6,9,11H,7-8,10H2,1-3H3
InchiKey:	CHAFAWKMYGLEPC-UHFFFAOYSA-N
Formula:	C13H20O
SMILES:	Cc1cccc(COCCC(C)C)c1
Mol. weight [g/mol]:	192.30

## Physical Properties

Property code	Value	Unit	Source
gf	53.92	kJ/mol	Joback Method
hf	-224.09	kJ/mol	Joback Method
hfus	20.74	kJ/mol	Joback Method
hvap	49.49	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.558		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	1411.00		NIST Webbook
rinpol	1411.00		NIST Webbook
tb	550.48	K	Joback Method
tc	750.64	K	Joback Method
tf	282.44	K	Joback Method
vc	0.667	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.77	J/molxK	550.48	Joback Method
cpg	438.01	J/molxK	583.84	Joback Method
cpg	454.39	J/molxK	617.20	Joback Method
cpg	469.93	J/molxK	650.56	Joback Method
cpg	484.66	J/molxK	683.92	Joback Method
cpg	498.59	J/molxK	717.28	Joback Method
cpg	511.75	J/molxK	750.64	Joback Method
dvisc	0.0026219	Paxs	282.44	Joback Method

dvisc	0.0011656	Paxs	327.11	Joback Method
dvisc	0.0006296	Paxs	371.79	Joback Method
dvisc	0.0003881	Paxs	416.46	Joback Method
dvisc	0.0002628	Paxs	461.13	Joback Method
dvisc	0.0001906	Paxs	505.81	Joback Method
dvisc	0.0001457	Paxs	550.48	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=U374586&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U374586&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.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>

## Legend

<b>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</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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