

# (3-Methylphenyl) methanol, n-pentyl ether

<b>Inchi:</b>	InChI=1S/C13H20O/c1-3-4-5-9-14-11-13-8-6-7-12(2)10-13/h6-8,10H,3-5,9,11H2,1-2H3
<b>InchiKey:</b>	DGQCCFUWTKWUDU-UHFFFAOYSA-N
<b>Formula:</b>	C13H20O
<b>SMILES:</b>	CCCCCOCc1ccc(C)c1
<b>Mol. weight [g/mol]:</b>	192.30

## Physical Properties

Property code	Value	Unit	Source
gf	56.36	kJ/mol	Joback Method
hf	-218.81	kJ/mol	Joback Method
hfus	24.27	kJ/mol	Joback Method
hvap	49.88	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.702		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2129.52	kPa	Joback Method
rinpol	1454.00		NIST Webbook
tb	550.92	K	Joback Method
tc	747.00	K	Joback Method
tf	297.44	K	Joback Method
vc	0.673	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.48	J/molxK	550.92	Joback Method
cpg	437.30	J/molxK	583.60	Joback Method
cpg	453.31	J/molxK	616.28	Joback Method
cpg	468.53	J/molxK	648.96	Joback Method
cpg	482.97	J/molxK	681.64	Joback Method
cpg	496.65	J/molxK	714.32	Joback Method
cpg	509.60	J/molxK	747.00	Joback Method
dvisc	0.0019570	Paxs	297.44	Joback Method
dvisc	0.0009863	Paxs	339.69	Joback Method

dvisc	0.0005784	Paxs	381.93	Joback Method
dvisc	0.0003773	Paxs	424.18	Joback Method
dvisc	0.0002659	Paxs	466.43	Joback Method
dvisc	0.0001986	Paxs	508.67	Joback Method
dvisc	0.0001551	Paxs	550.92	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U374440&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U374440&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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