

# m-Toluic acid, 3-methylbutyl ester

<b>Other names:</b>	Benzoic acid, 3-methyl-, 3-methylbutyl ester
<b>Inchi:</b>	InChI=1S/C13H18O2/c1-10(2)7-8-15-13(14)12-6-4-5-11(3)9-12/h4-6,9-10H,7-8H2,1-3H3
<b>InchiKey:</b>	LWJZTQRDMEFPX-UHFFFAOYSA-N
<b>Formula:</b>	C13H18O2
<b>SMILES:</b>	<chem>Cc1cccc(C(=O)OCCC(C)C)c1</chem>
<b>Mol. weight [g/mol]:</b>	206.28
<b>CAS:</b>	6640-76-2

## Physical Properties

Property code	Value	Unit	Source
gf	-75.00	kJ/mol	Joback Method
hf	-336.67	kJ/mol	Joback Method
hfus	22.34	kJ/mol	Joback Method
hvap	56.24	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.198		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	1573.00		NIST Webbook
tb	604.35	K	Joback Method
tc	812.28	K	Joback Method
tf	332.37	K	Joback Method
vc	0.673	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.45	J/molxK	604.35	Joback Method
cpg	459.38	J/molxK	639.01	Joback Method
cpg	474.43	J/molxK	673.66	Joback Method
cpg	488.62	J/molxK	708.32	Joback Method
cpg	501.96	J/molxK	742.97	Joback Method
cpg	514.48	J/molxK	777.63	Joback Method
cpg	526.19	J/molxK	812.28	Joback Method

dvisc	0.0020794	Paxs	332.37	Joback Method
dvisc	0.0010385	Paxs	377.70	Joback Method
dvisc	0.0006019	Paxs	423.03	Joback Method
dvisc	0.0003877	Paxs	468.36	Joback Method
dvisc	0.0002698	Paxs	513.69	Joback Method
dvisc	0.0001992	Paxs	559.02	Joback Method
dvisc	0.0001539	Paxs	604.35	Joback Method

## Sources

<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>
<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=C6640762&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6640762&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>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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