

# Butanoic acid, 3-methylphenyl ester

<b>Other names:</b>	Butyric acid, m-tolyl ester m-Cresyl butanoate Butyric acid, 3-methylphenyl ester
<b>Inchi:</b>	InChI=1S/C11H14O2/c1-3-5-11(12)13-10-7-4-6-9(2)8-10/h4,6-8H,3,5H2,1-2H3
<b>InchiKey:</b>	GYQSJJGXMUTZPU-UHFFFAOYSA-N
<b>Formula:</b>	C11H14O2
<b>SMILES:</b>	CCCC(=O)Oc1cccc(C)c1
<b>Mol. weight [g/mol]:</b>	178.23
<b>CAS:</b>	7476-80-4

## Physical Properties

Property code	Value	Unit	Source
gf	-89.40	kJ/mol	Joback Method
hf	-290.11	kJ/mol	Joback Method
hfus	20.69	kJ/mol	Joback Method
hvap	52.17	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.701		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
tb	559.03	K	Joback Method
tc	769.35	K	Joback Method
tf	324.83	K	Joback Method
vc	0.568	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.15	J/molxK	559.03	Joback Method
cpg	360.31	J/molxK	594.08	Joback Method
cpg	373.70	J/molxK	629.14	Joback Method
cpg	386.36	J/molxK	664.19	Joback Method
cpg	398.29	J/molxK	699.24	Joback Method
cpg	409.50	J/molxK	734.30	Joback Method

cpg	420.01	J/mol×K	769.35	Joback Method
dvisc	0.0017437	Paxs	324.83	Joback Method
dvisc	0.0009957	Paxs	363.86	Joback Method
dvisc	0.0006338	Paxs	402.90	Joback Method
dvisc	0.0004369	Paxs	441.93	Joback Method
dvisc	0.0003200	Paxs	480.96	Joback Method
dvisc	0.0002455	Paxs	520.00	Joback Method
dvisc	0.0001955	Paxs	559.03	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C7476804&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7476804&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>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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