

# 4-Butylbenzoic acid, 3-methylbut-2-yl ester

<b>Inchi:</b>	InChI=1S/C16H24O2/c1-5-6-7-14-8-10-15(11-9-14)16(17)18-13(4)12(2)3/h8-13H,5-7H2,
<b>InchiKey:</b>	JITREAXBTOGWSV-UHFFFAOYSA-N
<b>Formula:</b>	C16H24O2
<b>SMILES:</b>	CCCCc1ccc(C(=O)OC(C)C(C)C)cc1
<b>Mol. weight [g/mol]:</b>	248.36

## Physical Properties

Property code	Value	Unit	Source
gf	-52.18	kJ/mol	Joback Method
hf	-403.87	kJ/mol	Joback Method
hfus	26.59	kJ/mol	Joback Method
hvap	62.53	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.231		Crippen Method
mcvol	219.980	ml/mol	McGowan Method
pc	1771.36	kPa	Joback Method
rinsol	1842.00		NIST Webbook
tb	672.55	K	Joback Method
tc	875.45	K	Joback Method
tf	351.18	K	Joback Method
vc	0.836	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.65	J/molxK	672.55	Joback Method
cpg	618.31	J/molxK	706.37	Joback Method
cpg	634.95	J/molxK	740.18	Joback Method
cpg	650.60	J/molxK	774.00	Joback Method
cpg	665.29	J/molxK	807.82	Joback Method
cpg	679.05	J/molxK	841.64	Joback Method
cpg	691.90	J/molxK	875.45	Joback Method
dvisc	0.0022010	Paxs	351.18	Joback Method
dvisc	0.0009452	Paxs	404.74	Joback Method

dvisc	0.0004946	Paxs	458.30	Joback Method
dvisc	0.0002964	Paxs	511.87	Joback Method
dvisc	0.0001957	Paxs	565.43	Joback Method
dvisc	0.0001388	Paxs	618.99	Joback Method
dvisc	0.0001040	Paxs	672.55	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U354162&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354162&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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