

# Benzoic acid, 3-(3-methylbutyl)oxy-, methyl ester

Inchi:	InChI=1S/C13H18O3/c1-10(2)7-8-16-12-6-4-5-11(9-12)13(14)15-3/h4-6,9-10H,7-8H2,1-3
InchiKey:	GXLSHJZZYXOSOF-UHFFFAOYSA-N
Formula:	C13H18O3
SMILES:	<chem>COC(=O)c1cccc(OCCC(C)C)c1</chem>
Mol. weight [g/mol]:	222.28

## Physical Properties

Property code	Value	Unit	Source
gf	-180.00	kJ/mol	Joback Method
hf	-468.89	kJ/mol	Joback Method
hfus	23.53	kJ/mol	Joback Method
hvap	58.65	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.898		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	1684.00		NIST Webbook
tb	626.77	K	Joback Method
tc	832.59	K	Joback Method
tf	354.60	K	Joback Method
vc	0.692	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.86	J/molxK	626.77	Joback Method
cpg	485.46	J/molxK	661.07	Joback Method
cpg	500.22	J/molxK	695.38	Joback Method
cpg	514.14	J/molxK	729.68	Joback Method
cpg	527.21	J/molxK	763.98	Joback Method
cpg	539.46	J/molxK	798.29	Joback Method
cpg	550.88	J/molxK	832.59	Joback Method
dvisc	0.0014954	Paxs	354.60	Joback Method
dvisc	0.0007775	Paxs	399.96	Joback Method

dvisc	0.0004619	Paxs	445.32	Joback Method
dvisc	0.0003021	Paxs	490.69	Joback Method
dvisc	0.0002123	Paxs	536.05	Joback Method
dvisc	0.0001577	Paxs	581.41	Joback Method
dvisc	0.0001222	Paxs	626.77	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=U375320&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U375320&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>

## 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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