

# Benzoic acid, 4-(3-methylbutyl)amino-, methyl ester

Inchi:	InChI=1S/C13H19NO2/c1-10(2)8-9-14-12-6-4-11(5-7-12)13(15)16-3/h4-7,10,14H,8-9H2,
InchiKey:	RKDKMPLYJGJTQU-UHFFFAOYSA-N
Formula:	C13H19NO2
SMILES:	COC(=O)c1ccc(NCCC(C)C)cc1
Mol. weight [g/mol]:	221.30

## Physical Properties

Property code	Value	Unit	Source
gf	14.39	kJ/mol	Joback Method
hf	-283.20	kJ/mol	Joback Method
hfus	27.44	kJ/mol	Joback Method
hvap	62.67	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.931		Crippen Method
mcvol	187.690	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinsol	1957.00		NIST Webbook
tb	654.52	K	Joback Method
tc	862.27	K	Joback Method
tf	385.03	K	Joback Method
vc	0.709	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.02	J/mol×K	654.52	Joback Method
cpg	512.54	J/mol×K	689.15	Joback Method
cpg	527.14	J/mol×K	723.77	Joback Method
cpg	540.84	J/mol×K	758.40	Joback Method
cpg	553.67	J/mol×K	793.02	Joback Method
cpg	565.65	J/mol×K	827.65	Joback Method
cpg	576.80	J/mol×K	862.27	Joback Method

# Sources

<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=U375354&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U375354&amp;Units=SI</a>
<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>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>hvac:</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>mccol:</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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