

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

<b>Inchi:</b>	InChI=1S/C17H27NO2/c1-13(2)9-11-18-16-7-5-15(6-8-16)17(19)20-12-10-14(3)4/h5-8,1
<b>InchiKey:</b>	QEZATWMOKZSCRE-UHFFFAOYSA-N
<b>Formula:</b>	C17H27NO2
<b>SMILES:</b>	CC(C)CCNc1ccc(C(=O)OCCC(C)C)cc1
<b>Mol. weight [g/mol]:</b>	277.40

## Physical Properties

Property code	Value	Unit	Source
gf	45.63	kJ/mol	Joback Method
hf	-371.04	kJ/mol	Joback Method
hfus	34.28	kJ/mol	Joback Method
hvap	71.19	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.348		Crippen Method
mcvol	244.050	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
rinsol	2310.00		NIST Webbook
tb	745.60	K	Joback Method
tc	947.13	K	Joback Method
tf	415.11	K	Joback Method
vc	0.926	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.08	J/mol×K	745.60	Joback Method
cpg	732.26	J/mol×K	779.19	Joback Method
cpg	748.38	J/mol×K	812.78	Joback Method
cpg	763.48	J/mol×K	846.36	Joback Method
cpg	777.58	J/mol×K	879.95	Joback Method
cpg	790.71	J/mol×K	913.54	Joback Method
cpg	802.91	J/mol×K	947.13	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=U375460&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U375460&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>mccvol:</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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