

# Benzoic acid, 2-di(3-methylbutyl)amino-, 3-methylbutyl ester

<b>Inchi:</b>	InChI=1S/C22H37NO2/c1-17(2)11-14-23(15-12-18(3)4)21-10-8-7-9-20(21)22(24)25-16-1
<b>InchiKey:</b>	PFQDRNKAZZHSCC-UHFFFAOYSA-N
<b>Formula:</b>	C22H37NO2
<b>SMILES:</b>	CC(C)CCOC(=O)c1ccccc1N(CCC(C)C)CCC(C)C
<b>Mol. weight [g/mol]:</b>	347.53

## Physical Properties

Property code	Value	Unit	Source
gf	106.68	kJ/mol	Joback Method
hf	-465.46	kJ/mol	Joback Method
hfus	41.63	kJ/mol	Joback Method
hvap	77.54	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.788		Crippen Method
mcvol	314.500	ml/mol	McGowan Method
pc	1152.22	kPa	Joback Method
rinpola	2106.00		NIST Webbook
tb	821.83	K	Joback Method
tc	1019.18	K	Joback Method
tf	436.27	K	Joback Method
vc	1.183	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.88	J/molxK	821.83	Joback Method
cpg	1009.04	J/molxK	854.72	Joback Method
cpg	1027.01	J/molxK	887.61	Joback Method
cpg	1043.81	J/molxK	920.51	Joback Method
cpg	1059.50	J/molxK	953.40	Joback Method
cpg	1074.13	J/molxK	986.29	Joback Method
cpg	1087.75	J/molxK	1019.18	Joback Method

# Sources

<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=U375471&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U375471&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>

# 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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