

# Dibenzylamine, N-isoBOC

<b>Inchi:</b>	InChI=1S/C19H23NO2/c1-16(2)15-22-19(21)20(13-17-9-5-3-6-10-17)14-18-11-7-4-8-12-
<b>InchiKey:</b>	LJHBMKIDADLCHL-UHFFFAOYSA-N
<b>Formula:</b>	C19H23NO2
<b>SMILES:</b>	CC(C)COC(=O)N(Cc1ccccc1)Cc1ccccc1
<b>Mol. weight [g/mol]:</b>	297.39

## Physical Properties

Property code	Value	Unit	Source
gf	208.34	kJ/mol	Joback Method
hf	-144.98	kJ/mol	Joback Method
hfus	35.33	kJ/mol	Joback Method
hvap	73.25	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.481		Crippen Method
mcvol	248.470	ml/mol	McGowan Method
pc	1845.16	kPa	Joback Method
rinqol	2176.00		NIST Webbook
tb	775.77	K	Joback Method
tc	998.10	K	Joback Method
tf	446.36	K	Joback Method
vc	0.919	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.72	J/molxK	775.77	Joback Method
cpg	740.80	J/molxK	812.83	Joback Method
cpg	756.57	J/molxK	849.88	Joback Method
cpg	771.10	J/molxK	886.94	Joback Method
cpg	784.48	J/molxK	923.99	Joback Method
cpg	796.77	J/molxK	961.05	Joback Method
cpg	808.04	J/molxK	998.10	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=R392419&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R392419&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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