

# Benzoic acid, 4-isopropylamino-, isopropyl ester

Inchi:	InChI=1S/C13H19NO2/c1-9(2)14-12-7-5-11(6-8-12)13(15)16-10(3)4/h5-10,14H,1-4H3
InchiKey:	WCFCJMVEBHAUDB-UHFFFAOYSA-N
Formula:	C13H19NO2
SMILES:	CC(C)Nc1ccc(C(=O)OC(C)C)cc1
Mol. weight [g/mol]:	221.30

## Physical Properties

Property code	Value	Unit	Source
gf	11.95	kJ/mol	Joback Method
hf	-288.48	kJ/mol	Joback Method
hfus	23.92	kJ/mol	Joback Method
hvap	62.29	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.072		Crippen Method
mvol	187.690	ml/mol	McGowan Method
pc	2322.54	kPa	Joback Method
rinpol	1798.00		NIST Webbook
rinpol	1798.00		NIST Webbook
tb	654.08	K	Joback Method
tc	865.76	K	Joback Method
tf	370.03	K	Joback Method
vc	0.703	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.50	J/molxK	654.08	Joback Method
cpg	513.34	J/molxK	689.36	Joback Method
cpg	528.23	J/molxK	724.64	Joback Method
cpg	542.17	J/molxK	759.92	Joback Method
cpg	555.20	J/molxK	795.20	Joback Method
cpg	567.33	J/molxK	830.48	Joback Method
cpg	578.60	J/molxK	865.76	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U375467&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U375467&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>hvpap:</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>rinppl:</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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