

# 4-Chlorobenzamide, N-(4-chlorobenzoyl)-N-isobutyl-

<b>Inchi:</b>	InChI=1S/C18H17Cl2NO2/c1-12(2)11-21(17(22)13-3-7-15(19)8-4-13)18(23)14-5-9-16(20)
<b>InchiKey:</b>	CSHZQFDWUCFPEP-UHFFFAOYSA-N
<b>Formula:</b>	C18H17Cl2NO2
<b>SMILES:</b>	CC(C)CN(C(=O)c1ccc(Cl)cc1)C(=O)c1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	350.24

## Physical Properties

Property code	Value	Unit	Source
gf	132.88	kJ/mol	Joback Method
hf	-159.12	kJ/mol	Joback Method
hfus	40.77	kJ/mol	Joback Method
hvap	85.45	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	4.932		Crippen Method
mvol	254.560	ml/mol	McGowan Method
pc	1964.82	kPa	Joback Method
rinpol	2440.00		NIST Webbook
rinpol	2440.00		NIST Webbook
tb	869.16	K	Joback Method
tc	1109.23	K	Joback Method
tf	547.67	K	Joback Method
vc	0.950	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.03	J/molxK	869.16	Joback Method
cpg	713.54	J/molxK	909.17	Joback Method
cpg	724.95	J/molxK	949.18	Joback Method
cpg	735.34	J/molxK	989.19	Joback Method
cpg	744.81	J/molxK	1029.20	Joback Method
cpg	753.45	J/molxK	1069.22	Joback Method
cpg	761.35	J/molxK	1109.23	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=U407102&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407102&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>h vap:</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>r in pol:</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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