

# Benzamide, N-(2-iodo-4-methylphenyl)-4-chloro-

**Inchi:** InChI=1S/C14H11ClINO/c1-9-2-7-13(12(16)8-9)17-14(18)10-3-5-11(15)6-4-10/h2-8H,1H

**InchiKey:** YYP CJOSSNKECCK-UHFFFAOYSA-N

**Formula:** C14H11ClINO

**SMILES:** Cc1ccc(NC(=O)c2ccc(Cl)cc2)c(I)c1

**Mol. weight [g/mol]:** 371.60

## Physical Properties

Property code	Value	Unit	Source
gf	269.59	kJ/mol	Joback Method
hf	108.38	kJ/mol	Joback Method
hfus	34.23	kJ/mol	Joback Method
hvap	80.24	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.505		Crippen Method
mvol	210.210	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
rinpol	2630.00		NIST Webbook
rinpol	2630.00		NIST Webbook
tb	822.63	K	Joback Method
tc	1094.02	K	Joback Method
tf	528.51	K	Joback Method
vc	0.781	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.71	J/mol×K	822.63	Joback Method
cpg	511.86	J/mol×K	867.86	Joback Method
cpg	521.96	J/mol×K	913.09	Joback Method
cpg	531.11	J/mol×K	958.32	Joback Method
cpg	539.40	J/mol×K	1003.56	Joback Method
cpg	546.96	J/mol×K	1048.79	Joback Method
cpg	553.86	J/mol×K	1094.02	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U307401&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307401&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>hvp:</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>rinp:</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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