

# 3',4'-Dichloropivalanilide

<b>Inchi:</b>	InChI=1S/C11H13Cl2NO/c1-11(2,3)10(15)14-7-4-5-8(12)9(13)6-7/h4-6H,1-3H3,(H,14,15)
<b>InchiKey:</b>	WMFDYXPRRHDSQS-UHFFFAOYSA-N
<b>Formula:</b>	C11H13Cl2NO
<b>SMILES:</b>	CC(C)(C)C(=O)Nc1ccc(Cl)c(Cl)c1
<b>Mol. weight [g/mol]:</b>	246.13
<b>CAS:</b>	7160-22-7

## Physical Properties

Property code	Value	Unit	Source
gf	74.34	kJ/mol	Joback Method
hf	-156.12	kJ/mol	Joback Method
hfus	25.19	kJ/mol	Joback Method
hvap	64.34	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.978		Crippen Method
mcvol	178.120	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
tb	663.39	K	Joback Method
tc	896.72	K	Joback Method
tf	430.04	K	Joback Method
vc	0.671	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.22	J/molxK	663.39	Joback Method
cpg	436.83	J/molxK	702.28	Joback Method
cpg	448.48	J/molxK	741.17	Joback Method
cpg	459.23	J/molxK	780.05	Joback Method
cpg	469.13	J/molxK	818.94	Joback Method
cpg	478.27	J/molxK	857.83	Joback Method
cpg	486.69	J/molxK	896.72	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=C7160227&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7160227&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>hvap:</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>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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