

# 2,3-Dimethylbenzamide

<b>Inchi:</b>	InChI=1S/C9H11NO/c1-6-4-3-5-8(7(6)2)9(10)11/h3-5H,1-2H3,(H2,10,11)
<b>InchiKey:</b>	IZAYISYTIWLBNB-UHFFFAOYSA-N
<b>Formula:</b>	C9H11NO
<b>SMILES:</b>	<chem>Cc1cccc(C(N)=O)c1C</chem>
<b>Mol. weight [g/mol]:</b>	149.19
<b>CAS:</b>	5580-34-7

## Physical Properties

Property code	Value	Unit	Source
gf	55.58	kJ/mol	Joback Method
hf	-94.29	kJ/mol	Joback Method
hfus	19.13	kJ/mol	Joback Method
hvap	56.61	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	1.402		Crippen Method
mcvol	125.460	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
tb	568.36	K	Joback Method
tc	798.81	K	Joback Method
tf	375.84	K	Joback Method
vc	0.467	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.46	J/molxK	568.36	Joback Method
cpg	298.58	J/molxK	606.77	Joback Method
cpg	309.95	J/molxK	645.18	Joback Method
cpg	320.60	J/molxK	683.59	Joback Method
cpg	330.55	J/molxK	722.00	Joback Method
cpg	339.82	J/molxK	760.40	Joback Method
cpg	348.45	J/molxK	798.81	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=C5580347&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5580347&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>mccvol:</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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