

# 4-Dimethylamino-3,5-dinitrobenzoic acid

<b>Inchi:</b>	InChI=1S/C9H9N3O6/c1-10(2)8-6(11(15)16)3-5(9(13)14)4-7(8)12(17)18/h3-4H,1-2H3,(H
<b>InchiKey:</b>	HPESPZDCCQMDOO-UHFFFAOYSA-N
<b>Formula:</b>	C9H9N3O6
<b>SMILES:</b>	CN(C)c1c([N+](=O)[O-])cc(C(=O)O)cc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	255.18
<b>CAS:</b>	53639-29-5

## Physical Properties

Property code	Value	Unit	Source
gf	24.56	kJ/mol	Joback Method
hf	-245.77	kJ/mol	Joback Method
hfus	43.37	kJ/mol	Joback Method
hvap	98.54	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	1.267		Crippen Method
mcvol	166.170	ml/mol	McGowan Method
pc	3815.10	kPa	Joback Method
tb	909.11	K	Joback Method
tc	1151.05	K	Joback Method
tf	685.61	K	Joback Method
vc	0.638	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.82	J/molxK	909.11	Joback Method
cpg	486.08	J/molxK	949.43	Joback Method
cpg	492.63	J/molxK	989.76	Joback Method
cpg	498.50	J/molxK	1030.08	Joback Method
cpg	503.74	J/molxK	1070.40	Joback Method
cpg	508.40	J/molxK	1110.72	Joback Method
cpg	512.54	J/molxK	1151.05	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C53639295&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C53639295&amp;Units=SI</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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