

# 3,4-Difluoroaniline

<b>Other names:</b>	Benzenamine, 3,4-difluoro-
<b>Inchi:</b>	InChI=1S/C6H5F2N/c7-5-2-1-4(9)3-6(5)8/h1-3H,9H2
<b>InchiKey:</b>	AXNUZKSSQHTNPZ-UHFFFAOYSA-N
<b>Formula:</b>	C6H5F2N
<b>SMILES:</b>	<chem>Nc1ccc(F)c(F)c1</chem>
<b>Mol. weight [g/mol]:</b>	129.11
<b>CAS:</b>	3863-11-4

## Physical Properties

Property code	Value	Unit	Source
gf	-230.38	kJ/mol	Joback Method
hf	-312.01	kJ/mol	Joback Method
hfus	15.92	kJ/mol	Joback Method
hvap	53.30 ± 0.50	kJ/mol	NIST Webbook
log10ws	-1.77		Crippen Method
logp	1.547		Crippen Method
mcvol	85.160	ml/mol	McGowan Method
pc	4294.29	kPa	Joback Method
tb	470.00 ± 2.00	K	NIST Webbook
tc	652.54	K	Joback Method
tf	293.28	K	Joback Method
vc	0.329	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.45	J/mol×K	444.39	Joback Method
cpg	174.91	J/mol×K	479.08	Joback Method
cpg	182.90	J/mol×K	513.77	Joback Method
cpg	190.45	J/mol×K	548.47	Joback Method
cpg	197.56	J/mol×K	583.16	Joback Method
cpg	204.25	J/mol×K	617.85	Joback Method
cpg	210.54	J/mol×K	652.54	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	358.00	K	4.00	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3863114&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3863114&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>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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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