

# Benzenamine, 4-chloro-3-(trifluoromethyl)-

<b>Other names:</b>	5-Amino-2-chlorobenzotrifluoride 6-Chloro-3-aminobenzotrifluoride m-Toluidine, 4-chloro-«alpha», «alpha», «alpha»-trifluoro- Aniline, 4-chloro-3-(trifluoromethyl)- 3-(Trifluoromethyl)-4-chloroaniline 4-Chloro-3-(trifluoromethyl)aniline 4-chloro-«alpha», «alpha», «alpha»-trifluoro-m-toluidine
<b>Inchi:</b>	InChI=1S/C7H5ClF3N/c8-6-2-1-4(12)3-5(6)7(9,10)11/h1-3H,12H2
<b>InchiKey:</b>	ASPDJZINBYYZRU-UHFFFAOYSA-N
<b>Formula:</b>	C7H5ClF3N
<b>SMILES:</b>	Nc1ccc(Cl)c(C(F)(F)F)c1
<b>Mol. weight [g/mol]:</b>	195.57
<b>CAS:</b>	320-51-4

## Physical Properties

Property code	Value	Unit	Source
gf	-425.86	kJ/mol	Joback Method
hf	-553.25	kJ/mol	Joback Method
hfus	18.37	kJ/mol	Joback Method
hvap	46.06	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.941		Crippen Method
mcvol	113.260	ml/mol	McGowan Method
pc	3522.09	kPa	Joback Method
tb	500.74	K	Joback Method
tc	714.25	K	Joback Method
tf	337.48	K	Joback Method
vc	0.441	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.84	J/mol×K	500.74	Joback Method
cpg	249.38	J/mol×K	536.33	Joback Method

cpg	258.20	J/mol×K	571.91	Joback Method
cpg	266.33	J/mol×K	607.50	Joback Method
cpg	273.82	J/mol×K	643.08	Joback Method
cpg	280.71	J/mol×K	678.67	Joback Method
cpg	287.04	J/mol×K	714.25	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	358.00	K	0.40	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C320514&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C320514&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>
<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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