

# Benzenamine, 4-bromo-2-(trifluoromethyl)-

<b>Other names:</b>	2-Amino-5-bromobenzotrifluoride o-Toluidine, 4-bromo-«alpha», «alpha», «alpha»-trifluoro- 4-Bromo-2-(trifluoromethyl)aniline 4-Bromo-«alpha», «alpha», «alpha»-trifluoro-o-toluidine NSC 88311
<b>Inchi:</b>	InChI=1S/C7H5BrF3N/c8-4-1-2-6(12)5(3-4)7(9,10)11/h1-3H,12H2
<b>InchiKey:</b>	PHXGKHTWEOPCEW-UHFFFAOYSA-N
<b>Formula:</b>	C7H5BrF3N
<b>SMILES:</b>	Nc1ccc(Br)cc1C(F)(F)F
<b>Mol. weight [g/mol]:</b>	240.02
<b>CAS:</b>	445-02-3

## Physical Properties

Property code	Value	Unit	Source
gf	-399.61	kJ/mol	Joback Method
hf	-511.18	kJ/mol	Joback Method
h <sub>fus</sub>	19.46	kJ/mol	Joback Method
h <sub>vap</sub>	48.11	kJ/mol	Joback Method
log <sub>10</sub> ws	-3.37		Crippen Method
logp	3.050		Crippen Method
m <sub>cvol</sub>	118.520	ml/mol	McGowan Method
pc	4010.84	kPa	Joback Method
tb	529.47	K	Joback Method
tc	753.19	K	Joback Method
tf	367.36	K	Joback Method
vc	0.454	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
c <sub>pg</sub>	248.96	J/mol×K	529.47	Joback Method
c <sub>pg</sub>	258.25	J/mol×K	566.76	Joback Method
c <sub>pg</sub>	266.76	J/mol×K	604.04	Joback Method
c <sub>pg</sub>	274.55	J/mol×K	641.33	Joback Method

cpg	281.67	J/mol×K	678.62	Joback Method
cpg	288.17	J/mol×K	715.91	Joback Method
cpg	294.12	J/mol×K	753.19	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	358.20	K	0.70	NIST Webbook
tbrp	358.50 ± 0.50	K	0.70	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C445023&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C445023&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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