

# tert-Butyl

## N-(1-hydroxy-2,2,2-trifluoroethyl)carbamate

Inchi:	InChI=1S/C7H12F3NO3/c1-6(2,3)14-5(13)11-4(12)7(8,9)10/h4,12H,1-3H3,(H,11,13)
InchiKey:	HVTJYNRKBXOBCX-UHFFFAOYSA-N
Formula:	C7H12F3NO3
SMILES:	CC(C)(C)OC(=O)NC(O)C(F)(F)F
Mol. weight [g/mol]:	215.17
CAS:	17049-74-0

## Physical Properties

Property code	Value	Unit	Source
gf	-854.48	kJ/mol	Joback Method
hf	-1142.48	kJ/mol	Joback Method
hfus	16.75	kJ/mol	Joback Method
hvap	58.02	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	1.392		Crippen Method
mcvol	138.090	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
tb	569.11	K	Joback Method
tc	740.09	K	Joback Method
tf	345.90	K	Joback Method
vc	0.531	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.58	J/molxK	569.11	Joback Method
cpg	376.67	J/molxK	597.61	Joback Method
cpg	386.17	J/molxK	626.10	Joback Method
cpg	395.10	J/molxK	654.60	Joback Method
cpg	403.49	J/molxK	683.10	Joback Method
cpg	411.37	J/molxK	711.59	Joback Method
cpg	418.76	J/molxK	740.09	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C17049740&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C17049740&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>mcvol:</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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