

# 3,3,3-Trifluoroalanine

<b>Inchi:</b>	InChI=1S/C3H4F3NO2/c4-3(5,6)1(7)2(8)9/h1H,7H2,(H,8,9)
<b>InchiKey:</b>	HMJQKIDUCWWIBW-UHFFFAOYSA-N
<b>Formula:</b>	C3H4F3NO2
<b>SMILES:</b>	NC(C(=O)O)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	143.06

## Physical Properties

Property code	Value	Unit	Source
gf	-808.94	kJ/mol	Joback Method
hf	-938.63	kJ/mol	Joback Method
hfus	12.71	kJ/mol	Joback Method
hvap	52.20	kJ/mol	Joback Method
log10ws	-0.39		Crippen Method
logp	-0.039		Crippen Method
mcvol	75.860	ml/mol	McGowan Method
pc	5087.49	kPa	Joback Method
rinpol	840.00		NIST Webbook
rinpol	840.00		NIST Webbook
tb	480.76	K	Joback Method
tc	655.99	K	Joback Method
tf	306.77	K	Joback Method
vc	0.294	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.30	J/mol×K	480.76	Joback Method
cpg	186.16	J/mol×K	509.96	Joback Method
cpg	191.63	J/mol×K	539.17	Joback Method
cpg	196.73	J/mol×K	568.37	Joback Method
cpg	201.47	J/mol×K	597.58	Joback Method
cpg	205.89	J/mol×K	626.78	Joback Method
cpg	209.98	J/mol×K	655.99	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=R221857&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R221857&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>rinpola:</b>	Non-polar retention indices
<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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