

# Benzoic acid, 3-(trifluoroacetylamino)-

<b>Inchi:</b>	InChI=1S/C9H6F3NO3/c10-9(11,12)8(16)13-6-3-1-2-5(4-6)7(14)15/h1-4H,(H,13,16)(H,14)
<b>InchiKey:</b>	OWVHKHGMKQTLGA-UHFFFAOYSA-N
<b>Formula:</b>	C9H6F3NO3
<b>SMILES:</b>	O=C(O)c1ccccc(NC(=O)C(F)(F)F)c1
<b>Mol. weight [g/mol]:</b>	233.14
<b>CAS:</b>	4855-05-4

## Physical Properties

Property code	Value	Unit	Source
gf	-759.18	kJ/mol	Joback Method
hf	-925.03	kJ/mol	Joback Method
hfus	26.93	kJ/mol	Joback Method
hvap	71.43	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	1.886		Crippen Method
mcvol	138.210	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
rinpol	1656.00		NIST Webbook
rinpol	1656.00		NIST Webbook
tb	681.65	K	Joback Method
tc	878.18	K	Joback Method
tf	447.66	K	Joback Method
vc	0.540	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.15	J/molxK	681.65	Joback Method
cpg	371.11	J/molxK	714.41	Joback Method
cpg	378.45	J/molxK	747.16	Joback Method
cpg	385.19	J/molxK	779.92	Joback Method
cpg	391.40	J/molxK	812.67	Joback Method
cpg	397.10	J/molxK	845.43	Joback Method
cpg	402.33	J/molxK	878.18	Joback Method

# Sources

<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=C4855054&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4855054&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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>h vap:</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>r in pol:</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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