

# 2,3,6-Trifluorobenzamide

<b>Inchi:</b>	InChI=1S/C7H4F3NO/c8-3-1-2-4(9)6(10)5(3)7(11)12/h1-2H,(H2,11,12)
<b>InchiKey:</b>	BWWGEHSEZGXKEB-UHFFFAOYSA-N
<b>Formula:</b>	C7H4F3NO
<b>SMILES:</b>	NC(=O)c1c(F)ccc(F)c1F
<b>Mol. weight [g/mol]:</b>	175.11
<b>CAS:</b>	207986-22-9

## Physical Properties

Property code	Value	Unit	Source
gf	-555.32	kJ/mol	Joback Method
hf	-652.81	kJ/mol	Joback Method
hfus	22.80	kJ/mol	Joback Method
hvap	50.37	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	1.203		Crippen Method
mcvol	102.590	ml/mol	McGowan Method
pc	3815.10	kPa	Joback Method
tb	525.39	K	Joback Method
tc	731.08	K	Joback Method
tf	367.59	K	Joback Method
vc	0.408	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.20	J/molxK	525.39	Joback Method
cpg	232.23	J/molxK	559.67	Joback Method
cpg	239.81	J/molxK	593.95	Joback Method
cpg	246.96	J/molxK	628.23	Joback Method
cpg	253.67	J/molxK	662.52	Joback Method
cpg	259.97	J/molxK	696.80	Joback Method
cpg	265.86	J/molxK	731.08	Joback Method

# Sources

<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=C207986229&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C207986229&amp;Units=SI</a>
<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>

# 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>hvac:</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>mccol:</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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