

# 2,4,5-Trifluorobenzoic acid

<b>Other names:</b>	Benzoic acid, 2,4,5-trifluoro-
<b>Inchi:</b>	InChI=1S/C7H3F3O2/c8-4-2-6(10)5(9)1-3(4)7(11)12/h1-2H,(H,11,12)
<b>InchiKey:</b>	AKAMNXFLKYKFOJ-UHFFFAOYSA-N
<b>Formula:</b>	C7H3F3O2
<b>SMILES:</b>	O=C(O)c1cc(F)c(F)cc1F
<b>Mol. weight [g/mol]:</b>	176.09
<b>CAS:</b>	446-17-3

## Physical Properties

Property code	Value	Unit	Source
gf	-758.59	kJ/mol	Joback Method
hf	-838.83	kJ/mol	Joback Method
hfus	21.69	kJ/mol	Joback Method
hvap	56.41	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	1.802		Crippen Method
mcvol	98.480	ml/mol	McGowan Method
pc	3985.56	kPa	Joback Method
tb	545.04	K	Joback Method
tc	729.27	K	Joback Method
tf	345.15	K	Joback Method
vc	0.399	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.12	J/mol×K	545.04	Joback Method
cpg	222.66	J/mol×K	575.75	Joback Method
cpg	228.86	J/mol×K	606.45	Joback Method
cpg	234.74	J/mol×K	637.16	Joback Method
cpg	240.29	J/mol×K	667.86	Joback Method
cpg	245.53	J/mol×K	698.57	Joback Method
cpg	250.46	J/mol×K	729.27	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C446173&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C446173&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>
<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>hvp:</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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