

# Benzoic acid, 6-furfurylamino-3-sulfamoyl-4-trifluoromethyl-

<b>Inchi:</b>	InChI=1S/C13H11F3N2O5S/c14-13(15,16)9-5-10(18-6-7-2-1-3-23-7)8(12(19)20)4-11(9)2
<b>InchiKey:</b>	VJXQIJOREQDNBE-UHFFFAOYSA-N
<b>Formula:</b>	C13H11F3N2O5S
<b>SMILES:</b>	NS(=O)(=O)c1cc(C(=O)O)c(NCc2ccco2)cc1C(F)(F)F
<b>Mol. weight [g/mol]:</b>	364.30
<b>CAS:</b>	17642-12-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.19		Crippen Method
logp	2.256		Crippen Method
mcvol	217.480	ml/mol	McGowan 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>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=C17642125&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C17642125&amp;Units=SI</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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