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

Inchi: 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

InchiKey: VJXQIJOREQDNBE-UHFFFAOYSA-N

Formula: C13H11F3N2O5S

SMILES: NS(=O)(=O)c1cc(C(=O)O)c(NCc2ccco2)cc1C(F)(F)F

Mol. weight [g/mol]: 364.30

CAS: 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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17642125&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume