4-amino-N-(5-ethyl-1,3,4-thiadiazol-2-yl)benzenesu

Inchi: InChI=1S/C10H12N4O2S2/c1-2-9-12-13-10(17-9)14-18(15,16)8-5-3-7(11)4-6-8/h3-6H,2,

InchiKey: SVYBEBLNQGDRHF-UHFFFAOYSA-N

Formula: C10H12N4O2S2

SMILES: CCc1nnc(NS(=O)(=O)c2ccc(N)cc2)s1

Mol. weight [g/mol]: 284.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.21		Aqueous Solubility Prediction Method
logp	1.484		Crippen Method
mcvol	192.900	ml/mol	McGowan Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume