4-amino-N-(5-propan-2-yl-1,3,4-thiadiazol-2-yl)ben

Inchi: InChI=1S/C11H14N4O2S2/c1-7(2)10-13-14-11(18-10)15-19(16,17)9-5-3-8(12)4-6-9/h3-7
InchiKey: OPIGMRDAPFQALU-UHFFFAOYSA-N
Formula: C11H14N4O2S2
SMILES: CC(C)c1nnc(NS(=O)(=O)c2ccc(N)cc2)s1
Mol. weight [g/mol]: 298.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.41		Aqueous Solubility Prediction Method
logp	2.044		Crippen Method
mcvol	206.990	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

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