4-(ethylamino)-2-(3-methoxypropyl)-1,1-dioxo-3,4-

Inchi: InChI=1S/C12H21N3O5S3/c1-3-14-10-8-15(5-4-6-20-2)23(18,19)12-9(10)7-11(21-12)22(

InchiKey: HCRKCZRJWPKOAR-UHFFFAOYSA-N

Formula: C12H21N3O5S3

SMILES: CCNC1CN(CCCOC)S(=O)(=O)c2sc(S(N)(=O)=O)cc21

Mol. weight [g/mol]: 383.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.95		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	0.087		Crippen Method
mcvol	257.960	ml/mol	McGowan Method

Sources

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

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