

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/ci9903071>

Legend

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

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