3-[(5-methyl-1,3,4-thiadiazol-2-yl)sulfanylmethyl]-8 acid

Inchi: InChI=1S/C14H14N8O4S3/c1-6-17-18-14(29-6)28-4-7-3-27-12-9(11(24)22(12)10(7)13(25

InchiKey: MLYYVTUWGNIJIB-UHFFFAOYSA-N

Formula: C14H14N8O4S3

SMILES: Cc1nnc(SCC2=C(C(=O)O)N3C(=O)C(NC(=O)Cn4cnnn4)C3SC2)s1

Mol. weight [g/mol]: 454.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.62		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	-0.636		Crippen Method
mcvol	282.650	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