4-Methyl-N-((4-methyl-1-piperazinyl)carbonyl)-ben N-methyl-

Inchi: InChI=1S/C14H21N3O3S/c1-12-4-6-13(7-5-12)21(19,20)16(3)14(18)17-10-8-15(2)9-11-1

InchiKey: KZROTBBUPVAVKY-UHFFFAOYSA-N

Formula: C14H21N3O3S

SMILES: Cc1ccc(S(=O)(=O)N(C)C(=O)N2CCN(C)CC2)cc1

Mol. weight [g/mol]: 311.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.50		Crippen Method
logp	0.983		Crippen Method
mcvol	233.100	ml/mol	McGowan Method
rinpol	2435.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374390&Units=SI

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

rinpol: Non-polar retention indices

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