N-(P-AMINOPHENYLSULFONYL)-N-(3,4-DIMETHY

Other names: Acetamide, N-(3,4-dimethyl-5-isoxazolyl)-N-sulfanilyl-
Acetamide, N-[(4-aminophenyl)sulfonyl]-N-(3,4-dimethyl-5-isoxazolyl)-
Acetyl sulfisoxazole
Lipo Gantrisin
N-(3,4-Dimethyl-5-isoxazolyl)-N-sulfanilylacetamide
N-3,4-dimethylisoxazol-5-yl-N-sulphanilylacetamide

Inchi: InChI=1S/C13H15N3O4S/c1-8-9(2)15-20-13(8)16(10(3)17)21(18,19)12-6-4-11(14)5-7-12

InchiKey: JFNWFXVFBDDWCX-UHFFFAOYSA-N

Formula: C13H15N3O4S

SMILES: CC(=O)N(c1onc(C)c1C)S(=O)(=O)c1ccc(N)cc1

Mol. weight [g/mol]: 309.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Aqueous Solubility Prediction Method
logp	1.615		Crippen Method
mcvol	216.280	ml/mol	McGowan Method
tf	466.65	K	Aqueous Solubility Prediction Method

Sources

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C80740

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point