N-(5-METHYL-3-ISOXAZOLYL)-N-SULFANILYLAC

Inchi: InChI=1S/C12H13N3O4S/c1-8-7-12(14-19-8)15-20(17,18)11-5-3-10(4-6-11)13-9(2)16/h3
InchiKey: GXPIUNZCALHVBA-UHFFFAOYSA-N
Formula: C12H13N3O4S
SMILES: CC(=O)Nc1ccc(S(=O)(=O)Nc2cc(C)on2)cc1
Mol. weight [g/mol]: 295.32

Physical Properties

Property code	Value	Unit	Source
ie	8.12	eV	Cheméo Relay (1.0)
log10ws	-2.80		Cheméo Relay (1.0)
logp	1.742		Crippen Method
mcvol	202.190	ml/mol	McGowan Method
tb	671.17	K	Cheméo Relay (1.0)
tf	478.57	K	Cheméo Relay (1.0)

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21312107&Units=SI

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point