4-Nitro-N-(4-p-tolyl-thiazol-2-yl)-benzenesulfonam
N-methyl-

Inchi: InChI=1S/C17H15N3O4S2/c1-12-3-5-13(6-4-12)16-11-25-17(18-16)19(2)26(23,24)15-9-

InchiKey: UNUZALSGLSUWHO-UHFFFAOYSA-N

Formula: C17H15N3O4S2

SMILES: Cc1ccc(-c2csc(N(C)S(=O)(=O)c3ccc([N+](=O)[O-])cc3)n2)cc1

Mol. weight [g/mol]: 389.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.13		Crippen Method
logp	3.852		Crippen Method
mcvol	265.230	ml/mol	McGowan Method
rinpol	3212.00		NIST Webbook
rinpol	3212.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374812&Units=SI

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.