

4-Nitro-N-(4-p-tolyl-thiazol-2-yl)-benzenesulfonamide

Inchi: InChI=1S/C16H13N3O4S2/c1-11-2-4-12(5-3-11)15-10-24-16(17-15)18-25(22,23)14-8-6-
InchiKey: DRCWRKIFOBIOQG-UHFFFAOYSA-N
Formula: C16H13N3O4S2
SMILES: Cc1ccc(-c2csc(NS(=O)=O)c3ccc([N+](=O)[O-])cc3)n2)cc1
Mol. weight [g/mol]: 375.42
CAS: 330593-31-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.23		Crippen Method
logp	3.828		Crippen Method
mcvol	251.140	ml/mol	McGowan Method
rinpol	3581.00		NIST Webbook
rinpol	3581.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C330593312&Units=SI>

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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