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

Inchi: InChI=1S/C16H13N3O2S/c1-11-2-4-12(5-3-11)15-10-22-16(18-15)17-13-6-8-14(9-7-13)1
InchiKey: OPPQDLHBTCIRSR-UHFFFAOYSA-N
Formula: C16H13N3O2S
SMILES: Cc1ccc(-c2csc(Nc3ccc([N+](=O)[O-])cc3)n2)cc1
Mol. weight [g/mol]: 311.36
CAS: 1326862-51-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.53		Crippen Method
logp	4.770		Crippen Method
mcvol	223.050	ml/mol	McGowan Method
rinpol	2824.00		NIST Webbook
rinpol	2824.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C1326862514&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