3-(3-Nitroanilinomethyl)-2-benzothiazolinethione

Other names: 2-Benzothiazolinethione, 3-[(m-nitroanilino)methyl]-
Inchi: InChI=1S/C14H11N3O2S2/c18-17(19)11-5-3-4-10(8-11)15-9-16-12-6-1-2-7-13(12)21-14
InchiKey: QXJUHNJHOMXNDT-UHFFFAOYSA-N
Formula: C14H11N3O2S2
SMILES: O=[N+]([O-])c1cccc(NCn2c(=S)sc3ccccc32)c1
Mol. weight [g/mol]: 317.39
CAS: 65537-00-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.11		Crippen Method
logp	4.410		Crippen Method
mcvol	215.520	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C65537000&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume