

Tizanidine

Other names:

2,1,3-Benzothiadiazole, 5-chloro-4-(2-imidazolin-2-ylamino)-
2,1,3-Benzothiadiazole-4-amine, 5-chloro-N-(4,5-dihydro-1H-imidazol-2-yl)-
5-Chloro-4-(2-imidazolin-2-ylamino)-2,1,3-benzothiadiazole
DS 103-282
Sirdalud
Ternelin

Inchi: InChI=1S/C9H8CIN5S/c10-5-1-2-6-8(15-16-14-6)7(5)13-9-11-3-4-12-9/h1-2H,3-4H2,(H2,
InchiKey: XFYDIVBRZNQMJC-UHFFFAOYSA-N
Formula: C9H8CIN5S
SMILES: Clc1ccc2nsnc2c1NC1=NCCN1
Mol. weight [g/mol]: 253.71
CAS: 51322-75-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.33		Crippen Method
logp	1.716		Crippen Method
mvol	162.080	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C51322759&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/21-649-8/Tizanidine.pdf>

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