Azosemide

Inchi: InChI=1S/C12H11ClN6O2S2/c13-9-5-10(15-6-7-2-1-3-22-7)8(12-16-18-19-17-12)4-11(9)
InchiKey: HMEDEBAJARCKCT-UHFFFAOYSA-N
Formula: C12H11ClN6O2S2
SMILES: NS(=O)(=O)c1cc(-c2nn[nH]n2)c(NCc2cccs2)cc1Cl
Mol. weight [g/mol]: 370.85
CAS: 27589-33-9

Physical Properties

Property code	Value	Unit	Source
logp	1.359		Crippen Method
mcvol	233.820	ml/mol	McGowan Method
tf	492.65	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Cheméo Relay (1.0, beta):

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0): https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

Latest version available from:

https://www.chemeo.com/cid/104-802-5/Azosemide.pdf

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