Nithiazide

Inchi: InChI=1S/C6H8N4O3S/c1-2-7-5(11)9-6-8-3-4(14-6)10(12)13/h3H,2H2,1H3,(H2,7,8,9,11)
InchiKey: FQSUTLQHSDLLAN-UHFFFAOYSA-N
Formula: C6H8N4O3S
SMILES: CCNC(=O)Nc1ncc([N+](=O)[O-])s1
Mol. weight [g/mol]: 216.22
CAS: 139-94-6

Physical Properties

Property code	Value	Unit	Source
logp	1.193		Crippen Method
mcvol	141.220	ml/mol	McGowan Method
tf	501.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

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):
Cheméo Relay (1.0, beta):

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/110-405-9/Nithiazide.pdf

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