sulfaquinoxaline

Inchi: InChI=1S/C14H12N4O2S/c15-10-5-7-11(8-6-10)21(19,20)18-14-9-16-12-3-1-2-4-13(12)1

InchiKey: NHZLNPMOSADWGC-UHFFFAOYSA-N

Formula: C14H12N4O2S

SMILES: Nc1ccc(S(=O)(=O)Nc2cnc3ccccc3n2)cc1

Mol. weight [g/mol]: 300.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Cheméo Relay (1.0)
logp	2.013		Crippen Method
mcvol	209.150	ml/mol	McGowan Method
tf	524.76	K	Cheméo Relay (1.0)

Sources

Solubilities of Sulfamethazine, Sulfadimethoxine, Sulfamethoxydiazine, Sulfamonomethoxine, Sulfamethoxazole, and Sulfaquinoxaline in 1-Octanol from (298.15 to 333.15) K: https://www.doi.org/10.1021/je800867a

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

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tf: Normal melting (fusion) point

Latest version available from:
https://www.chemeo.com/cid/102-070-0/sulfaquinoxaline.pdf