sulfamonomethoxine

Inchi: InChI=1S/C11H12N4O3S/c1-18-11-6-10(13-7-14-11)15-19(16,17)9-4-2-8(12)3-5-9/h2-7H
InchiKey: WMPXPUYPYQKQCX-UHFFFAOYSA-N
Formula: C11H12N4O3S
SMILES: COc1cc(NS(=O)(=O)c2ccc(N)cc2)ncn1
Mol. weight [g/mol]: 280.31

Physical Properties

Property code	Value	Unit	Source
hvap	119.04	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.73		Cheméo Relay (1.0)
logp	0.868		Crippen Method
mcvol	192.210	ml/mol	McGowan Method
tf	480.90	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

Solubilities of Sulfadiazine, Sulfamethazine, Sulfadimethoxine, Sulfamethoxydiazine, Sulfamonomethoxine, Sulfamethoxazole, and Sulfaquinoxaline in 1-Octanol from (298.15 to 333.15) K: https://www.doi.org/10.1021/je0603978

Solubilities of Sulfamethazine, Sulfadimethoxine, Sulfamonomethoxine, Sulfamethoxazole, and Sulfaquinoxaline in Water 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

Cheméo Relay (1.0): https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

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