Prazosin

Inchi: InChI=1S/C19H21N5O4/c1-26-15-10-12-13(11-16(15)27-2)21-19(22-17(12)20)24-7-5-23
InchiKey: IENZQIKPVFGBNW-UHFFFAOYSA-N
Formula: C19H21N5O4
SMILES: COc1cc2nc(N3CCN(C(=O)c4ccco4)CC3)nc(N)c2cc1OC
Mol. weight [g/mol]: 383.41
CAS: 19216-56-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.86		Cheméo Relay (1.0)
logp	1.785		Crippen Method
mcvol	274.110	ml/mol	McGowan Method
tf	555.15	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

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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