Proguanil

Inchi: InChI=1S/C11H16ClN5/c1-7(2)15-10(13)17-11(14)16-9-5-3-8(12)4-6-9/h3-7H,1-2H3,(H5,
InchiKey: SSOLNOMRVKKSON-UHFFFAOYSA-N
Formula: C11H16ClN5
SMILES: CC(C)N=C(N)N=C(N)Nc1ccc(Cl)cc1
Mol. weight [g/mol]: 253.74
CAS: 500-92-5

Physical Properties

Property code	Value	Unit	Source
ie	7.64	eV	Cheméo Relay (1.0)
log10ws	-4.36		Cheméo Relay (1.0)
logp	1.790		Crippen Method
mcvol	195.630	ml/mol	McGowan Method
tf	402.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

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):
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0): https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

ie: Ionization energy
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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