Mepirizole

Inchi: InChI=1S/C11H14N4O2/c1-7-5-9(16-3)13-11(12-7)15-10(17-4)6-8(2)14-15/h5-6H,1-4H3
InchiKey: RHAXSHUQNIEUEY-UHFFFAOYSA-N
Formula: C11H14N4O2
SMILES: COc1cc(C)nc(-n2nc(C)cc2OC)n1
Mol. weight [g/mol]: 234.26
CAS: 18694-40-1

Physical Properties

Property code	Value	Unit	Source
logp	1.296		Crippen Method
mcvol	174.290	ml/mol	McGowan Method
tf	364.15	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

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https://www.chemeo.com/cid/109-661-7/Mepirizole.pdf

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