

Pyrimidin-4-ol, 2-dimethylamino, 5,6-dimethyl

Inchi: InChI=1S/C8H13N3O/c1-5-6(2)9-8(11(3)4)10-7(5)12/h1-4H3,(H,9,10,12)
InchiKey: MUEHLDAHWSCFAG-UHFFFAOYSA-N
Formula: C8H13N3O
SMILES: Cc1nc(N(C)C)nc(O)c1C
Mol. weight [g/mol]: 167.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.41		Crippen Method
logp	0.865		Crippen Method
mcvol	135.630	ml/mol	McGowan Method
rinpol	1600.00		NIST Webbook
rinpol	1600.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R84598&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/36-909-3/Pyrimidin-4-ol-2-dimethylamino-5-6-dimethyl.pdf>

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