

2,3-Dimethyl-6,7-dihydro-5H-cyclopentapyrazine

Inchi: InChI=1S/C9H12N2/c1-6-7(2)11-9-5-3-4-8(9)10-6/h3-5H2,1-2H3
InchiKey: AIKNQWWUQFXNAZ-UHFFFAOYSA-N
Formula: C9H12N2
SMILES: Cc1nc2c(nc1C)CCC2
Mol. weight [g/mol]: 148.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.04		Crippen Method
logp	1.582		Crippen Method
mcvol	123.010	ml/mol	McGowan Method
rinpol	1202.00		NIST Webbook
rinpol	1202.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R219715&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/39-509-4/2-3-Dimethyl-6-7-dihydro-5H-cyclopentapyrazine.pdf>

Generated by Cheméo on 2024-04-19 21:07:17.7961084 +0000 UTC m=+15850086.716685711.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.