2,6-dimethyl-6,7-dihydro-5H-cyclopentapyrazine

Inchi: InChI=1S/C9H12N2/c1-6-3-8-9(4-6)11-7(2)5-10-8/h5-6H,3-4H2,1-2H3
InchiKey: FKMPZHRHBYPYIZ-UHFFFAOYSA-N
Formula: C9H12N2
SMILES: Cc1cnc2c(n1)CC(C)C2
Mol. weight [g/mol]: 148.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.74		Crippen Method
logp	1.520		Crippen Method
mcvol	123.010	ml/mol	McGowan Method
ripol	1718.00		NIST Webbook
ripol	1718.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R296772&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
ripol: Polar retention indices

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