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

Other names: 2-methyl-5H-6,7-dihydrocyclo- pentapyrazine
Inchi: InChI=1S/C8H10N2/c1-6-5-9-7-3-2-4-8(7)10-6/h5H,2-4H2,1H3
InchiKey: IMZGQUVGVWTFFY-UHFFFAOYSA-N
Formula: C8H10N2
SMILES: Cc1cnc2c(n1)CCC2
Mol. weight [g/mol]: 134.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	1.274		Crippen Method
mcvol	108.920	ml/mol	McGowan Method
rinpol	1179.00		NIST Webbook
rinpol	1179.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1188.00		NIST Webbook
ripol	1688.00		NIST Webbook
ripol	1688.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R221520&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

ripol: Polar retention indices