6,7-Dihydrocyclopentapyrazine

Inchi: InChI=1S/C7H8N2/c1-2-6-7(3-1)9-5-4-8-6/h4-5H,1-3H2
InchiKey: WCTDRGQIEULRBE-UHFFFAOYSA-N
Formula: C7H8N2
SMILES: c1cnc2c(n1)CCC2
Mol. weight [g/mol]: 120.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.08		Crippen Method
logp	0.965		Crippen Method
mcvol	94.830	ml/mol	McGowan Method
rinpol	1070.00		NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	1070.00		NIST Webbook
ripol	1619.00		NIST Webbook
ripol	1619.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R608076&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.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
ripol: Polar retention indices