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

Other names: 5-methyl-2,3-(«alpha»methyltrimethylene)pyrazine
Inchi: InChI=1S/C9H12N2/c1-6-3-4-8-9(6)11-7(2)5-10-8/h5-6H,3-4H2,1-2H3
InchiKey: BSJXUYSXMSRKHW-UHFFFAOYSA-N
Formula: C9H12N2
SMILES: Cc1cnc2c(n1)C(C)CC2
Mol. weight [g/mol]: 148.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.94		Crippen Method
logp	1.835		Crippen Method
mcvol	123.010	ml/mol	McGowan Method
rinpol	1243.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1243.00		NIST Webbook
ripol	1676.00		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1676.00		NIST Webbook
ripol	1680.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R236334&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices