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

Other names: 2,5-Dimethyl-6,7-dihydro-(5H)-cyclopentapyrazine
6,7-Dihydro-2,5-dimethyl-5H-cyclopentapyrazine
Inchi: InChI=1S/C9H12N2/c1-6-3-4-8-9(6)10-5-7(2)11-8/h5-6H,3-4H2,1-2H3
InchiKey: CTFGVWCFSGCLHZ-UHFFFAOYSA-N
Formula: C9H12N2
SMILES: Cc1cnc2c(n1)CCC2C
Mol. weight [g/mol]: 148.21
CAS: 38917-61-2

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	1220.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1225.00		NIST Webbook
rinpol	1220.00		NIST Webbook
ripol	1672.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C38917612&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