6-Methyl-2-pyrazinylmethanol

Inchi: InChI=1S/C6H8N2O/c1-5-2-7-3-6(4-9)8-5/h2-3,9H,4H2,1H3
InchiKey: NJBPQOAHJORLDU-UHFFFAOYSA-N
Formula: C6H8N2O
SMILES: Cc1cncc(CO)n1
Mol. weight [g/mol]: 124.14
CAS: 77164-93-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.62		Crippen Method
logp	0.277		Crippen Method
mcvol	97.470	ml/mol	McGowan Method
rinpol	1084.00		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=C77164933&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

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