

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

Inchi: InChI=1S/C9H12N2/c1-2-7-6-10-8-4-3-5-9(8)11-7/h6H,2-5H2,1H3
InchiKey: SKBYYPGTSFJLFF-UHFFFAOYSA-N
Formula: C9H12N2
SMILES: CCc1cnc2c(n1)CCC2
Mol. weight [g/mol]: 148.21

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.89 | | Crippen Method |
| logp | 1.528 | | Crippen Method |
| mcvol | 123.010 | ml/mol | McGowan Method |
| rinpola | 1196.00 | | NIST Webbook |
| rinpola | 1202.00 | | NIST Webbook |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R236512&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

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