

2,5-Bis(1-methylethyl)pyrazine

Other names: 2,5-Diisopropylpyrazine
Inchi: InChI=1S/C10H16N2/c1-7(2)9-5-12-10(6-11-9)8(3)4/h5-8H,1-4H3
InchiKey: LXJYUERPFWUCNN-UHFFFAOYSA-N
Formula: C10H16N2
SMILES: CC(C)c1cnc(C(C)C)cn1
Mol. weight [g/mol]: 164.25

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.37 | | Crippen Method |
| logp | 2.723 | | Crippen Method |
| mcvol | 147.960 | ml/mol | McGowan Method |
| rinpola | 1198.00 | | NIST Webbook |
| rinpola | 1198.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R402378&Units=SI>

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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