

# Pyrazine, (2-methylpentyl)-

|                      |                                                                          |
|----------------------|--------------------------------------------------------------------------|
| Other names:         | 2-methyl pentyl pyrazine                                                 |
| Inchi:               | InChI=1S/C10H16N2/c1-3-4-9(2)7-10-8-11-5-6-12-10/h5-6,8-9H,3-4,7H2,1-2H3 |
| InchiKey:            | UQDNAXJKOPOWKM-UHFFFAOYSA-N                                              |
| Formula:             | C10H16N2                                                                 |
| SMILES:              | CCCC(C)Cc1cnccn1                                                         |
| Mol. weight [g/mol]: | 164.25                                                                   |
| CAS:                 | 107697-81-4                                                              |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -3.24   |        | Crippen Method |
| logp          | 2.455   |        | Crippen Method |
| mcvol         | 147.960 | ml/mol | McGowan Method |
| rinpol        | 1240.00 |        | NIST Webbook   |
| rinpol        | 1240.00 |        | NIST Webbook   |
| rinpol        | 1240.00 |        | NIST Webbook   |
| ripol         | 1606.00 |        | NIST Webbook   |
| ripol         | 1606.00 |        | NIST Webbook   |

## Sources

|                 |                                                                                                                                                 |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C107697814&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C107697814&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                       |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                               |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                           |

## 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

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