

# Methyl pyrazine-2-carboxylate

|                             |                                                     |
|-----------------------------|-----------------------------------------------------|
| <b>Inchi:</b>               | InChI=1S/C6H6N2O2/c1-10-6(9)5-4-7-2-3-8-5/h2-4H,1H3 |
| <b>InchiKey:</b>            | TWII RMSFZNYMQE-UHFFFAOYSA-N                        |
| <b>Formula:</b>             | C6H6N2O2                                            |
| <b>SMILES:</b>              | COC(=O)c1cnccn1                                     |
| <b>Mol. weight [g/mol]:</b> | 138.13                                              |

## Physical Properties

| Property code | Value  | Unit   | Source             |
|---------------|--------|--------|--------------------|
| hvap          | 64.26  | kJ/mol | Cheméo Relay (1.0) |
| ie            | 9.52   | eV     | Cheméo Relay (1.0) |
| log10ws       | -0.48  |        | Cheméo Relay (1.0) |
| logp          | 0.263  |        | Crippen Method     |
| mcvol         | 99.040 | ml/mol | McGowan Method     |
| tb            | 490.21 | K      | Cheméo Relay (1.0) |
| tf            | 331.13 | K      | Cheméo Relay (1.0) |

## Sources

|                                  |                                                                                                                               |
|----------------------------------|-------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C6164790">http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C6164790</a> |
| <b>McGowan Method:</b>           | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>         |
| <b>Crippen Method:</b>           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                     |
| <b>Crippen Method:</b>           | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>             |
| <b>Cheméo Relay (1.0):</b>       |                                                                                                                               |
| <b>Cheméo Relay (1.0, beta):</b> |                                                                                                                               |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>ie:</b>      | Ionization energy                               |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |

**mcvol:** McGowan's characteristic volume  
**tb:** Normal Boiling Point Temperature  
**tf:** Normal melting (fusion) point

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