

# Propane, 2-bromo-1-methoxy

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C4H9BrO/c1-4(5)3-6-2/h4H,3H2,1-2H3 |
| <b>InchiKey:</b>            | PBHYCZIZMTYKAS-UHFFFAOYSA-N                 |
| <b>Formula:</b>             | C4H9BrO                                     |
| <b>SMILES:</b>              | COCC(C)Br                                   |
| <b>Mol. weight [g/mol]:</b> | 153.02                                      |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -110.32 | kJ/mol               | Joback Method  |
| hf            | -237.06 | kJ/mol               | Joback Method  |
| hfus          | 9.07    | kJ/mol               | Joback Method  |
| hvap          | 32.95   | kJ/mol               | Joback Method  |
| log10ws       | -1.13   |                      | Crippen Method |
| logp          | 1.416   |                      | Crippen Method |
| mcvol         | 90.590  | ml/mol               | McGowan Method |
| pc            | 4205.63 | kPa                  | Joback Method  |
| rinpol        | 742.00  |                      | NIST Webbook   |
| rinpol        | 742.00  |                      | NIST Webbook   |
| tb            | 379.06  | K                    | Joback Method  |
| tc            | 569.53  | K                    | Joback Method  |
| tf            | 201.87  | K                    | Joback Method  |
| vc            | 0.334   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 147.73    | J/molxK | 379.06          | Joback Method |
| cpg           | 155.59    | J/molxK | 410.81          | Joback Method |
| cpg           | 163.17    | J/molxK | 442.55          | Joback Method |
| cpg           | 170.47    | J/molxK | 474.30          | Joback Method |
| cpg           | 177.50    | J/molxK | 506.04          | Joback Method |
| cpg           | 184.26    | J/molxK | 537.79          | Joback Method |
| cpg           | 190.74    | J/molxK | 569.53          | Joback Method |
| dvisc         | 0.0043438 | Paxs    | 201.87          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0021239 | Paxs | 231.40 | Joback Method |
| dvisc | 0.0012210 | Paxs | 260.93 | Joback Method |
| dvisc | 0.0007856 | Paxs | 290.47 | Joback Method |
| dvisc | 0.0005483 | Paxs | 320.00 | Joback Method |
| dvisc | 0.0004067 | Paxs | 349.53 | Joback Method |
| dvisc | 0.0003160 | Paxs | 379.06 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R12056&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R12056&amp;Units=SI</a> |

## Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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